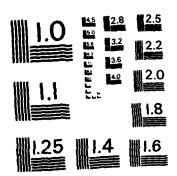
SPARSE MATRIX SOFTWARE CATALOG SPARSE MATRIX SYMPOSIUM 1982 FAIRFIELD GLADE TENNESSEE OCTOBER 24-27 1982(U) OAK RIDGE NATIONAL LAB IN M T HEATH 27 OCT 82 F/G 9/2 AD-A133 559 1/2 UNCLASSIFIED NL



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SOFTWARE CATA'LOG





SPARSE MATRIX SYMPOSIUM 1982

Fairfield Glade, Tennessee October 24-27, 1982



- U.S. Army Research Office
- U.S. Office of Naval Research
- Oak Ridge National Laboratory

(Mathematics and Statistics Research Department)

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SPARSE MATRIX SOFTWARE CATALOG

Sparse Matrix Symposium 1982

Fairfield Glade, Tennessee

October 24-27, 1982

Michael T. Heath, Editor

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Preface

This software catalog was prepared in conjunction with the Sparse Matrix Symposium in Fair-field Glade, Tennessee, October 25-27, 1982. It is intended to provide information on computer software for sparse matrix problems which should be useful to software developers and consumers alike. The information provided includes the problem domain to which the software is applicable, the method of solution, language and portability details, references to documentation, and a contact for further information or acquiring the software. This information is reported by means of a form which was filled out by each contributor for each item of software.

Contributions to the software catalog were solicited as part of the general announcement and call for papers for the Symposium which appeared in the official newsletters and other publications of several professional societies in mathematics, computer science, and operations research. There was also a mass mailing of general Symposium announcements to about 375 persons (mostly numerical analysts, applied mathematicians and computer scientists, plus a few engineers), and an additional mailing to about 80 persons which specifically solicited software catalog contributions. These efforts resulted in the submission of about 120 software forms. All submissions were accepted for inclusion in the catalog.

Thus, the catalog is about as complete as voluntary contributions can make it. In addition to containing virtually all of the software already well known to the sparse matrix community, many lesser-known packages are brought to light in these pages. The main area of sparse matrix software which is seriously underrepresented in the catalog is software for specific applications, such as structural analysis, in which modules which might have much wider applicability are buried within a much larger, special purpose package. We regret such omissions, but to have reached the practitioners in each of the diverse applications areas would have enormously expanded the scope of our publicity campaign and mailing lists.

The software reporting form which was sent to potential contributors was accompanied by a cover letter (which is reproduced here as Appendix A) and instructions for completing the form (Appendix B). In addition, the contributor was asked to help in organizing the catalog by specifying the appropriate categories and key words as outlined in Appendix C. There is also an appendix describing the restrictions on use of codes from the Harwell Subroutine Library, which its authors felt did not fit conveniently within the small space allowed for that purpose on the reporting form. The catalog is organized by problem domain and methods of solution, so that closely related programs appear near each other. As an aid in locating software by name of package or author, alphabetical indices are provided at the back of the catalog.

Most of the software forms have been photographically reproduced, exactly as received from the contributor. A few have been retyped for improved legibility (generally, those forms which were filled out by hand in pencil or colored ink). The accuracy of the information provided is therefore totally dependent on the individual contributors. The organizers and sponsors of the Symposium make no guarantee as to the accuracy of the information contained herein or the usefulness or validity of the software reported. The inclusion of information on a given item of software is not to be construed as an endorsement of it. It should be emphasized that this catalog is in no sense a software distribution service: in order to obtain any of the software discussed, the individual distributors listed on the forms must be contacted.

It is hoped that this catalog will provide a valuable service to the research and development community in the sparse matrix field and will also prove helpful to potential users in locating appropriate sparse matrix software. Perhaps it will become the basis for future efforts at even more comprehensive cataloging of software in sparse matrices as well as other areas.

Contents

1. Operations on Sparse Matrices	1
1.1 Multi-purpose packages	1
1.2 Products and scaling	
1.3 Permutations and transposition	
1.4 Assignment and block triangular form	
1.5 Bandwidth and profile reduction	
1.5 Bandwidth and profile reduction	18
1.6 Miscellaneous	19
2. Systems of Linear Equations	22
2.1 Direct methods	22
2.1.1 Nonsymmetric systems	22
2.1.1.1 General sparse matrices	22
2.1.1.2 Band or block forms	
2.1.2 Symmetric systems	
2.1.2.1 General sparse matrices	
2.1.2.2 Band or profile forms	
2.2 Iterative methods	
2.2.1 Multi-method package	
2.2.2 Gauss-Seidel and SOR	
2.2.3 Tchebychev	
2.2.4 Lanczos	
2.2.5 Preconditioned conjugate gradients	
2.2.6 Strongly implicit procedure	
	_
3. Least Squares Problems	73
3.1 Direct methods	7:
3.2 Iterative methods	70
4. Eigenvalue Problems	79
5. Optimization Problems	88
5.1 Linear programming	88
5.2 Nonlinear optimization	
5.2.1 Nonlinear equations	94
5.2.2 Unconstrained minimization	9:
5.2.3 Constrained minimization	
5.2.4 Jacobian and Hessian estimation	99
5.3 Miscellaneous applications	
6. Ordinary Differential Equations	104
7 Partial Differential Equations	111

Appendices	 12
Author Index	 12
Software Index	 12

1. Name of program or package: ALGORITHM 408

2. Descriptive title: A Sparse Matrix Package (Part 1)

3. Problem domain: (Elementary operations on general sparse matrices,

4. Method of solution: e.g., addition, multiplication, transposition,

extraction of rows.)

5. Programming language: FORTRAN 66

6. Precision: Single

7. Portability: Good (IBM 360)

8. Other packages required:

9. Mode of use: Subroutines

10. Test or demonstration program available?

11. Length of code in lines: ~ 1500 Percentage comments: 30%

12. Special features: -

13. Documentation and references: Comm. ACM 14 (1971), 265-273

Detailed header comments? ACM Trans. Math. Software 6 (1980), 456-457

User guide or manual, technical reports, papers, books:

14. Approximate cost of obtaining software: as per ACM TOMS rate

15. Restrictions on use: -

16. Distributor: ACM TOMS

17. Original source of software:
Developer: (See below)
Institution:
Sponsor:

18. For further information contact:

Professor J. M. McNamee Atkinson College, York University 4700 Keele Street Downsview, Ontario, CANADA M3J 2R7 1. Name of program or package: SPARSE

2. Descriptive title: Transformations and manipulations of sparse matrices

Linear algebra, arithmetic operations including 1/0, 3. Problem domain: transformations full matrices → sparse matrices,

transformations to NAG-routines Mark 5, 7

4. Method of solution: Inversion of part of a matrix via SOR-iteration inversion of a lower triangular matrix

5. Programming language: FORTRAN IV (FORTRAN 66) FORTRAN V (FORTRAN 77)

6. Precision: Depending on the hardware of the machine

7. Portability: PFORT-tested, special I/O in special modules

- 8. Other packages required:
- 9. Mode of use: Subroutine calls
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines:

Percentage comments: 20%

12. Special features: If the user is not familiar with the sparse techniques he can give full vectors or matrices and they are transformed automatically. Automatic use of disks (I/O) when the fields for the target matrices of

13. Documentation and references:

Detailed header comments? Yes

arithmetic operations are too small.

User guide or manual, technical reports, papers, books:

User guide at the moment only in German (70 pages) Base: J. M. McNamee's Algorithm 408, Comm. ACM $\underline{14}$ (1971), 265-273 U. Harms et al, TOMS, Vol. 6, No. 3, September 1980

14. Approximate cost of obtaining software: Noncommercial use: tape fee Commercial use: contact developer

15. Restrictions on use: None

16. Distributor: RRZN, Regionales Rechenzentrum für Niedersachsen, Wunstorfer Strasse 14

D-3000 Hannover 91, West Germany

17. Original source of software:

Developer: J. McNamee, U. Harms

Institution: RRZN

Sponsor:

18. For further information contact:

U. Harms RRZN Wunstorfer Strasse 14 D-3000 Hannover 91 West Germany

- 1. Name of program or package: RALAPACK
- 2. Descriptive title: Addition, multiplication, transposition, triangular factorization, backsubstitution, etc, with sparse matrices.
- 3. Problem domain: Real sparse matrices and vectors.
- 4. Method of solution: Sparse matrix techniques.
- 5. Programming language: FORTRAN IV.
- 6. Precision: Single.
- 7. Portability: IBM-360; IBM-370; VAX-11; CDC-6600; CDC-7600; XEROX-SIGMA-7. Easily portable to other machines.
- 8. Other packages required: None.
- 9. Mode of use: Callable subroutines.
- 10. Test or demonstration program available? No.
- 11. Length of code in lines: 388. Percentage comments: ---
- 12. Special features: None.

13. Documentation and references:

Detailed header comments? No

User guide or manual, technical reports, papers, books:

The operation manual is provided with the program (present version is in Spanish).

- 14. Approximate cost of obtaining software: None. Write to liaison officer.
- 15. Restrictions on use: Only for research purposes.
- **16. Distributor:** Liaison officer is: Sergio Pissanetzky, Centro Atómico Bariloche, 8400 Bariloche, R.N., Argentina.
- 17. Original source of software:

Developer: Sergio Pissanetzky

Institution: Comisión Nacional de Energía Atómica Sponsor: Comisión Nacional de Energía Atómica

18. For further information contact: ---

- 1. Name of program or package: SMULT
- 2. Descriptive title: Multiplies two sparse matrices together to form their

sparse product

- 3. Problem domain: General sparse matrices
- 4. Method of solution: Unordered merge and ordered merge
- 5. Programming language: FORTRAN
- 6. Precision: Single and double precision
- 7. Portability: IBM 370 in FORTRAN
- 8. Other packages required: Can use HALFP
- 9. Mode of use: Callable subroutine
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 400 lines Percentage comments: 50%
- **12. Special features:** Compute the product in the number of nontrivial multiplications
- 13. Documentation and references: Detailed header comments? \mathbf{Yes} User guide or manual, technical reports, papers, books:

Two Fast Algorithms for Sparse Matrices: Multiplication and Permuted Transposition, ACM TOMS, Vol. 4, September 1978, pp. 250-269

- 14. Approximate cost of obtaining software: See 18.
- 15. Restrictions on use: None
- 16. Distributor: Same as 18.
- 17. Original source of software:

Developer: Fred G. Gustavson

Institution: IBM Research

Sponsor:

18. For further information contact:

Dr. Fred G. Gustavson 33-205 IBM T. J. Watson Research Center P.O. Box 218

Yorktown Heights, New York 10598

Phone: (914) 945-1980

1. Name of program or package: PROD

2. Descriptive title: Obtain the product of two sparse matrices, or of a subset of the rows of ones times a subset of the columns of the second.

3. Problem domain: sparse matrices data management and operations

4. Method of solution: compares new indices of the first factor with column indices of the second.

5. Programming language: ANSI Standard Fortran

6. Precision: either

A NAME OF TAXABLE PARTY OF TAXABLE PARTY.

7. Portability: developed on a Cyber but very portable

8. Other packages required: none

9. Mode of use: callable subroutine

10. Test or demonstration program available? yes

11. Length of code in lines: 80 Percentage comments: 40%

12. Special features: different options of storage use are available, depending on the size of the matrices

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books: none at the present time

14. Approximate cost of obtaining software: free

15. Restrictions on use: none

16. Distributor: same as 18

17. Original source of software:

Developer: Daniel Szyld and Oleg Vishnepolsky

Institution: Institute for Economic Analysis-New York University

Sponsor:

18. For further information contact:

Daniel B. Szyld
Institute for Economic Analysis

New York University 269 Mercer Street New York, NY 10003

Phone (212) 598 3413

- **SPRSBLAS** 1. Name of program or package:
- 2. Descriptive title: Sparse vector operations on the CRAY-1.
- 3. Problem domain: Gather, scatter, dot and saxpy for sparse vectors. Also contains single and complex BLAS.
- 4. Method of solution: Standard algorithms optimized for CRAY-1, fastest available.
- 5. Programming language: CRAY-1 Assembler Language (CAL).
- 6. Precision: Single and complex.
- 7. Portability: Not portable.
- 8. Other packages required: These routines are a part of CRAYPACK (60 subroutines
- including BLAS, FFTS, sorting).
 Mode of use: FORTRAN-callable subroutines and functions.
- 10. Test or demonstration program available? No
- 11. Length of code in lines: 1000 lines Percentage comments: 30%
- 12. Special features: Software has been optimized to take advantage of CRAY-1 hardware.
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books: MAINSTREAM-EKS/VSP CRAYPACK Supplement to BCSLIB Users Manual.

- 14. Approximate cost of obtaining software: CRAYPACK is available to BCS network users.
- Possibility of sale to interested organizations is under review. 15. Restrictions on use:
- Use on BCS systems or if sold, internal use only. May not be distributed to others.

 16. Distributor: Boeing Computer Services Company
- 17. Original source of software:

Developer:

D. S. Dodson

Institution: Sponsor:

Boeing Computer Services Company Boeing Computer Services Company

18. For further information contact:

Kenneth W. Neves

Boeing Computer Services Company 565 Andover Park West, MS 9C-01

Tukwila, WA 98188 (206) 575-5074

1. Name of program or package: MC19

2. Descriptive title: Scales a sparse matrix.

3. Problem domain: Sparse matrices.

4. Method of solution: Minimizes the sum of squares of the logarithms of the non-zeros.

5. Programming language: IBM Fortran.

6. Precision: Both single and double precision versions are available.

7. Portability: Fortran 66 version available.

8. Other packages required: None.9. Mode of use: Subroutine calls.

5. Widde of use. Subfoutine cans.

10. Test of demonstration program available: Yes.

11. Length of code in lines: 174 Percentage comments: 24%

12. Special features:

13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

A.R.Curtis and J.K.Reid (1972) On the automatic scaling of matrices for Gaussian elimination. J. Inst. Math. Applics, **10**, 118–124.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (i), (ii), (iii), (iv) (see appendix on Harwell Subroutine Library).
- **16. Distributor:** S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.

17. Original source of software:

Developer: J.K.Reid.

Institution: A.E.R.E. Harwell. Sponsor: A.E.R.E. Harwell.

1. Name of program or package: HALFP

2. Descriptive title: Computes the transpose of PA where P is a permutation

matrix and A is sparse

3. Problem domain: Used to reorder the rows and columns of a sparse matrix

(form PAQ)

4. Method of solution: Distribution count sort

5. Programming language: FORTRAN

6. Precision: Single and double precision

7. Portability: IBM 370 in FORTRAN

8. Other packages required: None

9. Mode of use: Callable subroutine

10. Test or demonstration program available? Yes

11. Length of code in lines: 120 lines Percentage comments: 50%

12. Special features:

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

Two Fast Algorithms for Sparse Matrices: Multiplication and Permuted Transposition, ACM TOMS, Vol. 4, September 1978, pp. 250-269

- 14. Approximate cost of obtaining software: See 18.
- 15. Restrictions on use: None
- 16. Distributor: Same as 18.

17. Original source of software:

Developer: Fred G. Gustavson IBM Research

Sponsor:

18. For further information contact:

Dr. Fred G. Gustavson 33-205 IBM T. J. Watson Research Center P.O. Box 218 Yorktown Heights, New York 10598 Phone: (914) 945-1980

- 1. Name of program or package: TRANS
- 2. Descriptive title: to permute the rows (if matrix stored row wise) and transpose a sparse matrix, so large that only one fits in core.
- 3. Problem domain: sparse matrix data management
- 4. Method of solution: distribution of non zeros among row queues
- 5. Programming language: ANSI Standard Fortran
- 6. Precision: either

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- 7. Portability: developed on a Cyber, but very portable
- 8. Other packages required: none
- 9. Mode of use: callable subroutine
- 10. Test or demonstration program available? yes
- 11. Length of code in lines: 150

Percentage comments: 25%

- 12. Special features: writes output directly into secondary storage.
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

none at present time

- 14. Approximate cost of obtaining software: free
- 15. Restrictions on use: none
- 16. Distributor: same as 18
- 17. Original source of software:

Developer: Oleg Vishnepolsky

Institution: Institute for Economic Analysis, New York University

Sponsor:

18. For further information contact: Daniel B. Szyld

Institute for Economic Analysis

New York University 269 Mercer Street New York, NY 10003 Phone (212) 598 3413

- 1. Name of program or package: MC22
- 2. Descriptive title: Permutes a sparse matrix.
- 3. Problem domain: Sparse matrices.
- 4. Method of solution:

- 5. Programming language: IBM Fortran.
- 6. Precision: Both single and double precision versions are available.
- 7. Portability: Fortran 66 version available.
- 8. Other packages required: None.
- 9. Mode of use: Subroutine calls.
- 10. Test of demonstration program available: Yes.
- 11. Length of code in lines: 78 Percentage comments: 35%
- 12. Special features: Complex version (ME22) available.
- 13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii), (iii) (see appendix on Harwell Subroutine Library).
- **16. Distributor:** S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.
- 17. Original source of software:

Developer: I.S.Duff.

Institution: A.E.R.E. Harwell. Sponsor: A.E.R.E. Harwell.

1. Name of program or package: MC20

2. Descriptive title: Sorts non-zeros.

3. Problem domain: Sparse matrices.

4. Method of solution: In place sort by columns, handling each non-zero just once.

5. Programming language: IBM Fortran.

6. Precision: Both single and double precision versions are available.

7. Portability: Fortran 66 version available.

8. Other packages required: None.

9. Mode of use: Subroutine calls.

10. Test of demonstration program available: Yes.

11. Length of code in lines: 103

Percentage comments: 33%

12. Special features: Optional second entry bubble-sorts each column.

13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii), (iii) (see appendix on Harwell Subroutine Library).
- 16. Distributor: S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.

17. Original source of software:

Developer: A.W.Westerberg and J.K.Reid.

Institution: A.E.R.E. Harwell. Sponsor: A.E.R.E. Harwell.

18. For further information contact: J.K.Reid.

1. Name of program or package: SUBMAT

2. Descriptive title: Submatrices and/or row and column permutations of a

sparse matrix

3. Problem domain: Sparse Matrix data management

4. Method of solution: See 12

5. Programming language: ANSI standard FORTRAN

6. Precision: Either

7. Portability: Developed on IBM, used on a Cyber, Portable IBM version with half word integers also avaiable

8. Other packages required: None

9. Mode of use: Callable subroutine

10. Test or demonstration program available? Yes

11. Length of code in lines: 75

Percentage comments: 40%

12. Special features: If one considers the indicators for a subset of rows (or columns) as an application, say A: $R^n \to R^m$, the code uses the inverse application B: Rank (A) $\to R^n$

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

Proceedings, of the "I Jormadas Latinoamericanas de Matematica Aplicada" held in Santiago, Chile, December 1981

- 14. Approximate cost of obtaining software: Free
- 15. Restrictions on use: None
- 16. Distributor: Same as 18

17. Original source of software:

Developer: Daniel B. Szyld

institution: Institute for Economic Analysis, New York University

Sponsor:

18. For further information contact:

Daniel B. Szyld Institute for Economic Analysis New York University 269 Mercer Street New York, N.Y. 10003 Phone: (212) 598-3413

- 1. Name of program or package: FULL ASSIGN
- 2. Descriptive title: Compute a maximal assignment for an arbitrary
- 3. Problem domain: Arbitrary Sparse (0-1) Matrix
- **4. Method of solution:** The Assign Row Algorithm of Gustavson a modification of M. Hall's algorithm for finding an assignment
- 5. Programming language: APL, FORTRAN and 370 BAL versions
- 6. Precision: Single precision (only fixed point computations)
- 7. Portability: Standard ANSI FORTRAN
- 8. Other packages required: None

- 9. Mode of use: Callable FORTRAN subroutine
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: about 150 Percentage comments: about 60%
- 12. Special features: Fast and 100% accurate
- 13. Documentation and references:

 Detailed header comments? Yes

 User guide or manual, technical reports, papers, books:

Finding the Block Lower Triangular Form of a Sparse Matrix - Sparse Matrix Computations, J. R. Bunch and D. J. Rose (eds.) Academic Press, 1976, pp. 275-289

- 14. Approximate cost of obtaining software: See 18.
- 15. Restrictions on use: None
- 16. Distributor: Same as 18.
- 17. Original source of software:

Developer: Fred G. Gustavson IBM Research

Sponsor:

18. For further information contact:

Dr. Fred G. Gustavson 33-205 IBM T. J. Watson Research Center P.O. Box 218 Yorktown Heights, New York 10598 Phone: (914) 945-1980 1. Name of program or package: MC21

2. Descriptive title: Find a permutation to place non-zeros on the diagonal.

3. Problem domain: Sparse matrices.

4. Method of solution: Depth-first search with look-ahead.

5. Programming language: IBM Fortran.

6. Precision: Not applicable, since it works on the sparsity pattern.

7. Portability: Fortran 66 version available.

8. Other packages required: None.

9. Mode of use: Subroutine calls.

10. Test of demonstration program available: Yes.

11. Length of code in lines: 118 Percentage comments: 31%

12. Special features:

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13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

I.S.Duff (1981) On algorithms for obtaining a maximum transversal. A.C.M. Trans. Math. Software, 7, 315–330 and 387–390.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii), (iii) (see appendix on Harwell Subroutine Library).
- **16. Distributor:** S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.

17. Original source of software:

Developer: I.S.Duff.

Institution: A.E.R.E. Harwell. **Sponsor:** A.E.R.E. Harwell.

1. Name of program or package: BLTF

2. Descriptive title: Compute the block lower triangular form of a Sparse

Matrix

3. Problem domain:

4. Method of solution: A new improved version of Tarjan's Strong Connect Algorithm

5. Programming language: APL, FORTRAN and 370 BAL

6. Precision: Single precision7. Portability: Standard FORTRAN

8. Other packages required: None

9. Mode of use: Callable FORTRAN subroutine
10. Test or demonstration program available? Yes

11. Length of code in lines: About 150 Percentage comments: About 60%

12. Special features: Fast and 100% accurate

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

Finding the Block Lower Triangular Form of a Sparse Matrix - Sparse Matrix Computations, J. R. Bunch and D. J. Rose (eds.) Academic Press, 1976, pp. 275-289

- 14. Approximate cost of obtaining software: See 18.
- 15. Restrictions on use: None
- 16. Distributor: Same as 18.

17. Original source of software:

Developer: Fred G. Gustavson IEM Research
Sponsor:

18. For further information contact:

Dr. Fred G. Gustavson 33-205 IBM T. J. Watson Research Center P.O. Box 218 Yorktown Heights, New York 10598 Phone: (914) 945-1980

- 1. Name of program or package: MC13
- 2. Descriptive title: Finds a symmetric permutation for block triangular form.
- 3. Problem domain: Sparse matrices.
- 4. Method of solution: Tarjan's algorithm.
- 5. Programming language: IBM Fortran.
- 6. Precision: Not applicable, since it works on the sparsity pattern.
- 7. Portability: Fortran 66 version available.
- 8. Other packages required: None.
- 9. Mode of use: Subroutine calls.
- 10. Test of demonstration program available: Yes.
- 11. Length of code in lines: 131

Percentage comments: 46%

- 12. Special features:
- 13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

R.Tarjan (1972) Depth first search and linear graph algorithms. S.I.A.M. J. Comput. 1. 146–160.

I.S.Duff and J.K.Reid (1978) An implementation of Tarjan's algorithm for the block triangularization of a matrix. A.C.M. Trans. Math. Software 4, 137–147 and 189–192.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii), (iii) (see appendix on Harwell Subroutine Library).
- 16. Distributor: S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England, or I.M.S.L. (TOMS algorithm).
- 17. Original source of software:

Developer: I.S.Duff

Institution: A.E.R.E. Harwell. Sponsor: A.E.R.E. Harwell.

1. Name of program or package: MC23

2. Descriptive title: Permutes a sparse matrix to block triangular form.

3. Problem domain: Sparse matrices.

4. Method of solution: Uses Harwell routines MC13 and MC21.

5. Programming language: IBM Fortran

6. Precision: Both single and double precision versions are available.

7. Portability: Fortran 66 version available.

8. Other packages required: Harwell subroutines MC13, MC21.

9. Mode of use: Subroutine calls.

10. Test of demonstration program available: Yes.

11. Length of code in lines: 202 Percentage comments: 41%

(451 with dependencies)

12. Special features: Complex version (ME23) available.

13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii), (iii) (see appendix on Harwell Subroutine Library).
- 16. Distributor: S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.

17. Original source of software:

Developer: I.S.Duff.

Institution: A.E.R.E. Harwell. Sponsor: A.E.R.E. Harwell.

- 1. Name of program or package: GPSKCA, GPSKRA
- 2. Descriptive title: Bandwidth and profile (envelope) reduction.
- 3. Problem domain: Reordering algorithm for symmetric matrices.
- 4. Method of solution: Uses Gibbs-Poole, Stockmeyer and Gibbs-King algorithms.
- 5. Programming language: FORTRAN
- 6. Precision: Integer (nonzero values are not required; only locations).
- 7. Portability: Developed on CDC CYBER 760; portable.
- 8. Other packages required: None
- 9. Mode of use: Subroutine

- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 2500 lines Percentage comments: 50%
- 12. Special features: GPSKCA uses compact (linked lists) data format; GPSKRA uses rectangular array for connection table. Improved version of Algorithms 508, 509 (TOMS, December 1976). These new codes appeared in TOMS (June 1982).
- 13. Documentation and references: Detailed header comments? Yes User guide or manual, technical reports, papers, books: Description appeared in TOMS (June 1982).
- 14. Approximate cost of obtaining software: Standard TOMS fee.
- 15. Restrictions on use: None
- 16. Distributor: ACM TOMS
- 17. Original source of software:

Developer: J.G. Lewis modified 508, 509 (developed by Crane, Gibbs, Poole, Stockmeyer).

Institution: Boeing Computer Services Company Sponsor: Boeing Computer Services Company

18. For further information contact:

J.G. Lewis

Boeing Computer Services Company 565 Andover Park West, MS 9C-01

Tukwila, WA 98188 (206) 575-5102

- 1. Name of program or package:
- 2. Descriptive title:
- 3. Problem domain: Packing of the integer (index) vectors and matrices of the NAG Sparse routines
- 4. Method of solution:
- 5. Programming language: FORTRAN 66
- 6. Precision:
- 7. Portability: Only the packing routines are machine dependent, the packing is done by subroutine calls or function calls
- 8. Other packages required: NAG Library
- 9. Mode of use: Subroutine calls
- 10. Test or demonstration program available?
- 11. Length of code in lines:

Percentage comments:

- 12. Special features:
- 13. Documentation and references:
 Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

User guide but only in German at the moment Sparse Matrices and their Uses, I. S. Duff (ed.) Academic Press, London (1981) pp. 335-341

- 14. Approximate cost of obtaining software:
- 15. Restrictions on use: Contracts with NAG
- 16. Distributor:
- 17. Original source of software:

Developer: U. Harms Institution: RRZN Sponsor:

18. For further information contact:

U. Harms RRZN Wunstorfer Strasse 14 D-3000 Hannover 91 West Germany

- 1. Name of program or package: VMSYST
- 2. Descriptive title: Numerical data management system
- 3. Problem domain: General purpose support large volumes of data
- 4. Method of solution: Page buffering; "Least recently used" paging algorithm
- 5. Programming language: FORTRAN 66
- 6. Precision: NA

- 7. Portability: Good (Currently operational on: VAX 11/780, UNIVAC 11XX)
- 8. Other packages required: DMGASP (or suitable I/O interface)
- 9. Mode of use: Subroutine calls
- 10. Test or demonstration program available? Included
- 11. Length of code in lines: 1800 Percentage comments: 0
- **12. Special features:** Manages mass storage as a "virtual" word addressable memory or as a record file; Maintains file descriptive header; has a "note" (text) stack system.
- 13. Documentation and references:

 Petalled bander comments?

 Practic

Detailed header comments? Practically none in code User guide or manual, technical reports, papers, books:

"Supplementary Studies on the Sensitivity of Optimized Structures," AFWAL-TR-81-3013, National Technical Information Service (NTIS), 425 13th St., N.W., Washington, D.C. (March 1981).

- 14. Approximate cost of obtaining software: \$300
- 15. Restrictions on use: Not to be re-distributed
- 16. Distributor: Lockheed Research Lab.
- 17. Original source of software:

Developer: Paul S. Jensen

Institution: Lockheed Palo Alto Research Laboratory
Sponsor: AFOSR, ONERA, Lockheed Ind. Research

18. For further information contact:

Paul S. Jensen Lockheed Research Lab. 5233/255 3251 Hanover St. Palo Alto, CA 94304 1. Name of program or package: FFTPACK

2. Descriptive title: Subprograms for the fast Fourier transform of real, complex and symmetric sequences

3. Problem domain: Real, complex and symmetric sequences

4. Method of solution: Stockham auto-sort algorithm

5. Programming language: ANSI FORTRAN

6. Precision: Single

7. Portability: Developed on the Cray-1 but is easily ported

8. Other packages required: None

9. Mode of use: Subprogram

10. Test or demonstration program available? Yes

11. Length of code in lines: 2,000 Percentage comments: 30%

12. Special features: Nineteen subprograms for the fast transform of real, complex, real-even, real-odd and quarter wave transforms

13. Documentation and references: Yes, included with package Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

Paul N. Swartztrauber, Vectorizing the FFT's, in <u>Parallel Computations</u>, Garry Rodrigue (ed.) Academic Press, 1982

- 14. Approximate cost of obtaining software: \$300
- 15. Restrictions on use: None
- 16. Distributor: Scientific Computing Division

National Center for Atmospheric Research P.O. Box 3000, Boulder, Colorado 80307

17. Original source of software: Same as 16.

Developer: Paul N. Swartztrauber

Institution: NCAR Sponsor: NSF

18. For further information contact:

To order, contact Sue Long, NCAR (303) 494-5151, Ext. 505 or FTS 322-5505 Questions to Paul N. Swartztrauber (303) 494-5151, Ext. 605 or FTS 322-5605.

1. Name of program or package: F01BRF/A

2. Descriptive title: Decomposes a real sparse matrix

3. Problem domain: Real, linear equations.

4. Method of solution: LU decomposition

5. Programming language: FORTRAN and Algol 60

6. Precision: Either

7. Portability: Available on 48 machine ranges/compliers

8. Other packages required: NAG

9. Mode of use: Callable subroutine

10. Test or demonstration program available? Yes

11. Length of code in lines: 294 Percentage comments: 50%

12. Special features:

13. Documentation and references: Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

NAG Library Manual NAG On-line Supplement

- 14. Approximate cost of obtaining software: NAG Library costs \$1584/year
- 15. Restrictions on use: License agreement
- **16. Distributor:** NAG (U.S.A.) Inc. (see below)

17. Original source of software:

Developer: Dr. I. Duff Harwell (U.K.)
Sponsor: NAG

18. For further information contact:

Mrs. Carolyn M. Smith NAG (U.S.A.) Inc. 1250 Grace Court Downers Grove, IL 60516 Tel. 971-2337 Telex 23254708 (Teleserv DFLD) 1. Name of program or package: F01BSF/A

2. Descriptive title: Decomposes a real sparse matrix using pivotal sequence

previously determined

3. Problem domain: Real, linear, algebraic equations

4. Method of solution: LU decomposition

5. Programming language: FORTRAN and Algol 60

6. Precision: Either

7. Portability: Available on 48 machine ranges/compiler

8. Other packages required: NAG

9. Mode of use: Callable subroutine

10. Test or demonstration program available? Yes

11. Length of code in lines: 132 Percentage comments: 50%

12. Special features:

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

NAG Library Manual NAG On-line Supplement

- 14. Approximate cost of obtaining software: NAG Library costs \$1584/year
- 15. Restrictions on use: License agreement
- **16. Distributor:** NAG (U.S.A.) Inc. (see below)

17. Original source of software:

Developer: Dr. I. Duff Harwell (U.K.)
Sponsor: NAG

18. For further information contact:

The state of the s

Mrs. Carolyn M. Smith NAG (U.S.A.) Inc. 1250 Grace Court Downers Grove, IL 60516 Tel. 971-2337 Telex 23254708 (Telesery DFLD) 1. Name of program or package: F04AXF/A

2. Descriptive title: Solves a system of linear equations

3. Problem domain: Real, sparse, linear algebraic equations

4. Method of solution: LU decomposition

5. Programming language: FORTRAN and Algol 60

6. Precision: Either

7. Portability: Available on 48 machine ranges/compliers

8. Other packages required: NAG

9. Mode of use: Callable subroutine

10. Test or demonstration program available? Yes

11. Length of code in lines: 42 Percentage comments: 75%

12. Special features:

13. Documentation and references:

Detailed header comments?

Yes

User guide or manual, technical reports, papers, books:

NAG Library Manual NAG On-line Supplement

- 14. Approximate cost of obtaining software: NAG Library costs \$1584/year
- 15. Restrictions on use: License agreement
- **16. Distributor:** NAG (U.S.A.) Inc. (see below)
- 17. Original source of software:

Developer: Dr. I. Duff Harwell Sponsor: NAG

18. For further information contact:

Mrs. Carolyn M. Smith
NAG (U.S.A.) Inc.
1250 Grace Court
Downers Grove, IL 60516
Tel. 971-2337
Telex. 23254708 (Telesery DFLD)

1. Name of program or package: MA28/MA30

2. Descriptive title: Solves linear sets of equations.

3. Problem domain: Sparse unsymmetric matrices.

4. Method of solution: LU decomposition, using Markowitz' pivoting.

5. Programming language: IBM Fortran.

6. Precision: Both single and double precision versions are available.

7. Portability: Fortran 66 version available.

- 8. Other packages required: Harwell subroutines MC13, MC20, MC21, MC22, MC23, MC24.
- 9. Mode of use: Subroutine calls.

- 10. Test of demonstration program available: Yes.
- 11. Length of code in lines: 1842 Percentage comments: 37%

(2520 with dependencies)

12. Special features: Includes automatic recognition of block triangular form. Complex version (ME28/ME30) available. Direct entry available (MA30/ME30) for sorted matrices.

13. Documentation and references:

Detailed header comments? Yes.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

I.S.Duff and J.K.Reid (1979), A.C.M. Trans. on Math. Software, 5, 18-35.

I.S.Duff (1977), MA28 – A set of Fortran subroutines for sparse unsymmetric linear equations. Harwell report R-8730, H.M.S.O., London.

I.S.Duff (1981) A.C.M. Trans. Math. Software, 7, 505-511.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (i), (ii), (iii), (iv) (see appendix on Harwell Subroutine Library).
- 16. Distributor: S. Marlow, CSS Division, Building 8.9, A E.B.E. Harwell, Oxfordshire OX11 ORA, England.

17. Original source of software:

Developer: I.S.Duff

Institution: A.E.R.E. Harwell. Sponsor: A.E.R.E. Harwell.

- 1. Name of program or package: MA32
- 2. Descriptive title: Solves unsymmetric sets of linear equations.
- 3. Problem domain: Finite element or finite difference equations.
- 4. Method of solution: Frontal elimination.
- 5. Programming language: IBM and CRAY Fortran.
- 6. Precision: Double precision (IBM) and single precision (CRAY).
- 7. Portability: Written in Fortran 66 except for isolated direct-access i/o statements.
- 8. Other packages required: IBM version calls other Harwell routines to establish files.
- 9. Mode of use: Subroutine calls.
- 10. Test of demonstration program available: Yes.
- 11. Length of code in lines: 2211 Percentage comments: 45%

(2522 with dependencies)

- **12. Special features:** Allows problems to be input by rows or by finite elements. Uses direct access storage.
- 13. Documentation and references:

Detailed header comments? Yes, of auxiliary routines.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

I.S.Duff (1981) Design features of a code for solving sparse unsymmetric linear systems out-of-core. Harwell report CSS 89.

I.S.Duff (1981) MA32 – A package for solving sparse unsymmetric systems using the frontal method. Harwell report R-10079.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (i), (ii), (iii), (iv) (see appendix on Harwell Subroutine Library).
- **16. Distributor:** S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.
- 17. Original source of software:

Developer: I.S.Duff.

Institution: A.E.R.E. Harwell. **Sponsor:** A.E.R.E. Harwell.

1. Name of program or package: MC24

2. Descriptive title: Bounds the size of non-zeros encountered in Gaussian elimination.

3. Problem domain: Sparse LU decomposition.

4. Method of solution: Hadamard's inequality.

5. Programming language: IBM Fortran.

6. Precision: Both single and double precision versions are available.

7. Portability: Fortran 66 version available.

Other packages required: None
 Mode of use: Subroutine calls.

10. Test of demonstration program available: Yes.

11. Length of code in lines: 46 Percentage comments: 32%

12. Special features: Complex version (ME24) available.

13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

A.M.Erisman and J.K.Reid (1974) Monitoring the stability of the triangular factorization of a sparse matrix. Numer. Math. **22**, 183–186.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii), (iii) (see appendix on Harwell Subroutine Library).
- 16. Distributor: S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.

17. Original source of software:

Developer: I.S.Duff.

Institution: A.E.R.E. Harwell. Sponsor: A.E.R.E. Harwell.

1. Name of program or package: NSPFAC

2. Descriptive title: Sparse Linear Equation Solver

3. Problem domain: Nonsymmetric Sparse Linear Equations

- 4. Method of solution: Sparse Gaussian Elimination with threshold partial pivoting
- 5. Programming language: Fortran
- 6. Precision: Single or Double available (Separately)
- 7. Portability: Developed on DEC-10, IBM/360, CDC-6600 Easily portable to other machines
- 8. Other packages required: None
- 9. Mode of use: Callable subroutines
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 400 Percentage comments: 61%
- 12. Special features: None

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

- A. H. Sherman, Algorithm 533-NSPIV, A Fortran Subroutine for Sparse Gaussian Elimination with Partial Pivoting, <u>Trans. on Math Software 4</u> (Dec., 1978), pp. 391-398.
- A. H. Sherman, Algorithms for Sparse Gaussian Elimination with Partial Pivoting, Trans. on Math Software 4 (Dec. 1978), pp. 330-338.
- 14. Approximate cost of obtaining software: No Cost
- 15. Restrictions on use: None
- 16. Distributor: Andrew H. Sherman

Exxon Production Research Co.

P. O. Box 2189

17. Original source of Software: 77001 713/966-6376

Developer: Andrew H. Sherman

Institution: University of Texas at Austin

Sponsor: AFOSR

18. For further information contact:

Andrew H. Sherman Exxon Production Research Co. P. O. Box 2189 Houston, TX 77001

713/966-6376

1. Name of program or package: PORT Sparse Matrix Package

2. Descriptive title: Subroutines for solving sparse unsymmetric linear

systems have been added to the PORT library.

3. Problem domain: Systems of linear equations, real and complex,

nonsymmetric, sparse

4. Method of solution: Direct methods, some subroutines do minimum degree ordering, others do threshold pivoting for stability given an initial

ordering.

5. Programming language: FORTRAN

6. Precision: Single and double

7. Portability: As portable as PORT, checked by PFORT verifier

- 8. Other packages required: Core subroutines in PORT which are in public domain
- 9. Mode of use: Callable subroutines
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 8800 lines Percentage comments: 20%
- **12. Special features:** Has easy to use subroutines and subroutines for problems with a number of matrices all with the same zero structure. Permits function input of matrices.
- 13. Documentation and references:
 Detailed header comments? Yes
 User guide or manual, technical reports, papers, books:

User guide available

- 14. Approximate cost of obtaining software: \$75 to universities, one time charge
- 15. Restrictions on use: License agreement
- 16. Distributor: Until third version of PORT library is released for distribution contact - Linda Kaufman, Bell Labs, Room 2C-459, Murray Hill, N.J. 07974
- 17. Original source of software:

Developer: Linda Kaufman Bell Labs
Sponsor:

18. For further information contact:

Linda Kaufman Bell Labs Room 2C-459 Murray Hill, N.J. 07974 1. Name of program or package: SSLEST

2. Descriptive title: LU-decomposition of general sparse matrix

3. Problem domain: Solution of systems of linear equations

4. Method of solution: Gaussian elimination with pivoting using Markowitz-strategy involving stability checking and dropping tolerance

5. Programming language: FORTRAN

6. Precision: Single precision IBM

7. Portability: Uses INTEGER*2 to save space

8. Other packages required: NONE

9. Mode of use: Callable subroutines

10. Test or demonstration program available? NO

11. Length of code in lines: 750 lines Percentage comments: 10% comments

12. Special features: The features of using drop-tolerance, selecting different pivoting strategies and of modifying the stability check are available. 8 different modes of operation

13. Documentation and references:

Detailed header comments?

User guide or manual, technical reports, papers, books:

Users Guide available, require rep. NI-78-01, gives detailed information on use and examples

14. Approximate cost of obtaining software: 50 \$

15. Restrictions on use: Non-commercial

16. Distributor: Dept. for Numerical Analysis

Technical University of Denmark, Building 303

DK-2800 Lyngby, Denmark

17. Original source of software:

Developer: Z. Zlatev, V.A. Barker, P.G. Thomsen

Institution: Dept. of Numerical Analysis, Technical University of Denmark

Sponsor:

18. For further information contact: Per Grove Thomsen

Dept. for Numerical Analysis, Building 303

Technical University of Denmark, DK-2800 Lyngby

DENMARK, Tel. 881911 ext. 4373

- 1. Name of program or package: Y12M
- 2. Descriptive title: Sparse linear systems package
- 3. Problem domain: Unsymmetric linear systems
- **4. Method of solution:** Gaussian elimination with a generalized Markowitz strategy; iterative refinement as an option
- 5. Programming language: ANSI FORTRAN
- 6. Precision: Both single and double precision versions for the direct
- 7. Portability: Portable
- 8. Other packages required: None
- 9. Mode of use: Callable subroutines
- 10. Test or demonstration program available? Yes, several test-matrices generators
- 11. Length of code in lines: about 2000 Percentage comments: 10%
- 12. Special features: Multibanking option for the UNIVAC 1100 installations
- 13. Documentation and references:

Detailed header comments? No

User guide or manual, technical reports, papers, books:

"Y12M - Solution of Large and Sparse Systems of Linear Algebraic Equations", Lecture Notes in Computer Science, Vol. 121, Springer,

SIAM J. Numer. Anal. 17(1980), 19(1982); Comp. Chem. 4(1980), 5(1981)

- 14. Approximate cost of obtaining software: Free of charge
- 15. Restrictions on use: None
- **16. Distributor:** Recku (Regional Computing Centre at the University of Copenhagen)
- 17. Original source of software:

Developer: Z.Zlatev, J.Wasniewski and K.Schaumburg

Institution: Recku, Copenhagen

Sponsor: Danish Natural Science Research Council

18. For further information contact: J. Wasniewski, Regional Computing Centre

at the University of Copenhagen,

Vermundsgade 5, 2100 Copenhagen Ø

Tlf. 01 - 83 95 11

- 1. Name of program or package: General Sparse Solver (SYMFAC, NUMFAC AND BKSLVE)
- 2. Descriptive title: General sparse linear system solver
- 3. Problem domain: Unsymmetric linear equation solver
- 4. Method of solution: SYMFAC NUMFAC approach
- 5. Programming language: FORTRAN
- 6. Precision: Single and double precision
- 7. Portability: Standard FORTRAN
- 8. Other packages required:
- 9. Mode of use: Callable FORTRAN subroutines
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: about 500 Percentage comments: about 50%
- 12. Special features:

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

Some Results on Sparse Matrices, IBM Research Report 1980 "Some Basic Techniques for Solving Sparse Systems of Linear Equations," Sparse Matrices and their Applications, D. J. Rose and R. A. Willoughby (eds.) Plenum Press, 1972, pp. 41-52

- 14. Approximate cost of obtaining software: See 18.
- 15. Restrictions on use: None
- 16. Distributor: Same as 18.

17. Original source of software:

Developer: Fred G. Gustavson IBM Research

Sponsor:

18. For further information contact:

Dr. Fred G. Gustavson 33-205 IBM T. J. Watson Research Center P.O. Box 218 Yorktown Heights, New York 10598 Phone: (914) 945-1980 1. Name of program or package:

2. Descriptive title: Symbolic Generation of an Optimal Crout Algorithm

3. Problem domain: Unsymmetric linear equation solver

4. Method of solution: Compiled code approach

5. Programming language: FORTRAN

6. Precision: Single and double precision

7. Portability: Standard FORTRAN

8. Other packages required: None

9. Mode of use: Callable FORTRAN subroutines

10. Test or demonstration program available? Yes

11. Length of code in lines: 1000 lines Percentage comments: 30%

12. Special features:

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

"Symbolic Generation of an Optimal Crout Algorithm," J. ACM, January 1970

- 14. Approximate cost of obtaining software: See 18.
- 15. Restrictions on use:
- 16. Distributor: Same as 18.

17. Original source of software:

Developer: Fred G. Gustavson institution: IBM Research Sponsor:

18. For further information contact:

Dr. Fred G. Gustavson 33-205 IBM T. J. Watson Research Center P.O. Box 218 Yorktown Heights, New York 10598

Phone: (914) 945-1980

- 1. Name of program or package: SPAR/VECTOR
- 2. Descriptive title: General Sparse Solver for CRAY-1
- 3. Problem domain: Unsymmetric sparse matrices
- 4. Method of solution: LU factorization
- 5. Programming language: Fortran
- 6. Precision: 64-Bit
- 7. Portability: CRAY-1, CRAY-1S, CRAY X-MP, CYBER 205
- 8. Other packages required: None
- 9. Mode of use: Subroutine
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 700 Percentage comments: 20
- 12. Special features: Two-pass symbolic/numeric. From column-ordered symbolic matrix description and row and column permutation vectors, dense segments of columns are tagged for later processing in vector mode.
- 13. Documentation and references: Detailed header comments?

User guide or manual, technical reports, papers, books:

"A Collection of Sparse Matrix Solvers for the CRAY-1", Report #166, Systems Engineering Laboratory, University of Michigan, Ann Arbor, MI 48109; October, 1982.

- 14. Approximate cost of obtaining software: Send user tape
- 15. Restrictions on use: None
- 16. Distributor: See Below
- 17. Original source of software:

Developer: D.A. Calahan, Dept. of Elec. & Comp. Engineering Institution: University of Michigan, Ann Arbor, MI 48109; 313-763-0036 Sponsor: Air Force Office of Scientific Research

18. For further information contact: See Above

1. Name of program or package: SPAR/SC/CRAY

2. Descriptive title: General Sparse Solver for CRAY-1 by Loopless Scalar Code Generation

- 3. Problem domain: Unsymmetric highly sparse matrices
- 4. Method of solution: LU factorization
- 5. Programming language: Fortran and CRAY Assembly Language
- 6. Precision: 64-Bit
- 7. Portability: CRAY-1, CRAY-1S, CRAY X-MP
- 8. Other packages required: None
- 9. Mode of use: Stand-alone; easily modified to subroutine
- 10. Test or demonstration program available?
- 11. Length of code in lines: 1600 Percentage comments: 20
- 12. Special features: Two-pass symbolic/numeric. After special equation ordering to maximize local decoupling, loopless scalar code is generated in symbolic phase. Achieves 14-16 MFLOPS.
- 13. Documentation and references: Detailed header comments? NO

User guide or manual, technical reports, papers, books:
"A Collection of Sparse Matrix Solvers for the CRAY-1", Report #166, Systems Engineering Laboratory, University of Michigan, Ann Arbor, MI 48109; October, 1982.

- 14. Approximate cost of obtaining software: Send user tape
- 15. Restrictions on use: None
- 16. Distributor: See Below
- 17. Original source of software:

Developer: D.A. Calahan, Dept. of Elec. & Comp Engineering Institution: University of Michigan, Ann Arbor, MI 48139

Sponsor: Air Force Office of Scientific Research

18. For further information contact: See Above

- 1. Name of program or package: RUFS
- 2. Descriptive title: Sparse linear system solver
- 3. Problem domain: Real, unsymmetric linear systems
- 4. Method of solution: LU Decomposition
- 5. Programming language: Assembly Language FPS-164 Array Processor
- 6. Precision: 64-bit word
- 7. Portability: Developed for the FPS-164 Array Processor. A version also exists for the following FPS 38-bit Array Processors: FPS-100, AP-120B, AP-180V, and AP-190L.

 8. Other packages required: FPS-164 Math Library (APMATH64)
- 9. Mode of use: Callable subroutine
- 10. Test or demonstration program available? No
- 11. Length of code in lines: 1017 Percentage comments:
- 12. Special features: Takes advantage of the parallel, pipelined architecture of the FPS-164 Array Processor.
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

APMATH64 Reference Manual Floating Point Systems, Inc.

- 14. Approximate cost of obtaining software: This routine is included in the FPS-164 Math Library (APMATH64)15. Restrictions on use: License agreement required
- 16. Distributor: Floating Point Systems, Inc.

P.O. Box 23489

Portland, OR (503) 641-3151

17. Original source of software:

Developer: Ron Coleman Institution: Floating Point Systems, Inc. Sponsor: Floating Point Systems, Inc.

18. For further information contact:

Phil Vaughn Floating Point Systems, Inc. P.O. Box 23489

Portland, OR 97223

TLX: 360470 FLOATPOIN BEAV (503) 641-3151

1. Name of program or package: CUFS

2. Descriptive title: Sparse linear system solver

3. Problem domain: Complex, unsymmetric linear systems

4. Method of solution: LU Decomposition

5. Programming language: FPS-164 Array Processor

6. Precision: 64-bit word

7. Portability: Developed for the FPS-164 Array Processor. A version also exists for the following FPS 38-bit Array Processors:
FPS-100, AP-120B, AP-180V, and AP-190L.

8. Other packages required: FPS-164 Math Library (APMATH64)

9. Mode of use: Callable subroutine

10. Test or demonstration program available? No

11. Length of code in lines: 1212 Percentage comments: 70

12. Special features: Takes advantage of the parallel, pipelined architecture

of the FPS-164 Array Processor.

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

APMATH64 Reference Manual Floating Point Systems, Inc.

14. Approximate cost of obtaining software: This, routine is included in the FPS-164 Math Library (APMATH64).

15. Restrictions on use: License agreement required

16. Distributor: Floating Point Systems, Inc.

P.O. Box 23489 Portland, OR 97223

(503) 641-3151 **17. Original source of software:**

Developer: Ron Coleman

Institution: Floating Point Systems, Inc. Sponsor: Floating Point Systems, Inc.

18. For further information contact:

Phil Vaughn
Floating Point Systems, Inc.
P.O. Box 23489
Portland, OR 97223

(503) 641-3151 TLX: 360470 FLOATPOIN BEAV

1. Name of program or package: ECTLIB

2. Descriptive title: Subroutines for out-of-core solutions of large complex linear systems

3. Problem domain: The solving of large linear complex systems

4. Method of solution: Sherman-Morrison Updating formula

5. Programming language: FORTRAN IV

6. Precision: Single

7. Portability: CDC CYBER 170 Series

8. Other packages required: No 9. Mode of use: Stand Alone

10. Test or demonstration program available? Yes

11. Length of code in lines: 3530 Percentage comments:

12. Special features:

Į.

Applicable to both dense and sparse matrices that are to large to stored in core

13. Documentation and references:

Detailed header comments? No

User guide or manual, technical reports, papers, books:

NASA CR159142

14. Approximate cost of obtaining software: \$675.00

15. Restrictions on useino

16. Distributor: COSMIC

112 Barrow Hall, University of Georgia

Athens, GA 30602

17. Original source of software:

Developer: Elizabeth Yip

Institution: Boeing Commercial Airplane Co. Sponsor: NASA Langley Research Center

18. For further information contact:

Steve Horton COSMIC 404 542-3265

- 1. Name of program or package: SPAR2PAS
- 2. Descriptive title: Sparse linear equation solver by 2-pass approach
- 3. Problem domain: Unsymmetric linear systems, reorder equations
- 4. Method of solution: P4, HP (hierarchical partitioning), Gaussian elimination
- 5. Programming language: FORTRAN, mostly ANSI with few exceptions
- 6. Precision: Single7. Portability: Portable
- 8. Other packages required: None
- 9. Mode of use: Callable subroutines
- 10. Test or demonstration program available? No
- 11. Length of code in lines: ~ 4500 Percentage comments: 30%
- 12. Special features: Optionally, matrix is out-of-core, row at a time processing; reordering techniques especially suited for chemical process flowsheeting problems.
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

User guide forthcoming.
Mark A. Stadtherr and E. Steven Wood, "Sparse Matrix Methods for
Equation Based Chemical Process Flowsheeting: I. Reordering Phase,
II. Numerical Phase," preprints.

- 14. Approximate cost of obtaining software: Small fee
- 15. Restrictions on use: none
- 16. Distributor: Same as 18
- 17. Original source of software:

Developer: Mark A. Stadtherr University of Illinois

Sponsor: NSF

18. For further information contact:

Mark A. Stadtherr Chemical Engineering Department University of Illinois 1209 West California Street Urbana, Illinois 61801 Phone: 217-333-0275 1. Name of program or package: LINPACK

2. Descriptive title: Dense linear equation solver

3. Problem domain:

Linear systems for general, banded, symmetric indefinite, symmetric positive definite, triangular and tridiagonal; plus

QR and SVD for rectangular matrices.

4. Method of solution:

Direct matrix factorization

5. Programming language: Fortran

6. Precision: Single, double, complex and double complex

7. Portability: Fully portable

8. Other packages required: BLAS

9. Mode of use: Callable subroutines

10. Test or demonstration program available? Yes

11. Length of code in lines: Percentage comments: 50%

7000 lines in each precision

12. Special features: Column orientation for efficiency.

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

LINPACK Users' Guide, J. J. Dongarra, J. R. Bunch, C. B. Moler, G. W. Stewart, SIAM Pub., Philadelphia, 1979.

- 14. Approximate cost of obtaining software: \$75 handling fee
- 15. Restrictions on use: None
- 16. Distributor: National Energy Software Center IMSL, Inc.

Argonne National Laboratory 9700 South Cass Avenue

Sixth Floor, NBC Building 7500 Bellaire Boulevard Houston, TX 77036

Argonne, IL 60439

17. Original source of software:

Developer: Dongarra, Bunch, Moler, Stewart

Institution: Argonne National Laboratory, Univ. of California (San Diego), Univ.

Sponsor: of New Mexico, Univ. of Maryland

NSF & DOE

18. For further information contact:

Jack Dongarra Mathematics and Computer Science Div. Argonne National Laboratory Argonne, IL 60439 (312) 972-7246

ARPA: ANLAMS!Dongarra@UCB-C70

- 1. Name of program or package: PROFILE/U/CRAY
- 2. Descriptive title: Unsymmetric Banded and Profile Solvers for the CRAY-1
- 3. Problem domain: Unsymmetric banded and profile matrices
- 4. Method of solution: LU factorization
- 5. Programming language: CRAY assembly language
- 6. Precision: 64-Bit
- 7. Portability: CRAY-1, CRAY-1S, CRAY X-MP
- 8. Other packages required: None
- 9. Mode of use: Subroutine
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 2700 Percentage comments: 20
- 12. Special features: Compressed storage by rows or columns; no bandwidth restriction; achieves 100 MFLOPS with bandwidths greater than 40.
- 13. Documentation and references: Detailed header comments? No

User guide or manual, technical reports, papers, books:

"High Performance Banded and Profile Solvers for the CRAY-1: The Unsymmetric Case" Report #160, Systems Engineering Laboratory, University of Michigan, Ann Arbor, MI 48109; February, 1982.

- 14. Approximate cost of obtaining software: Send user tape
- 15. Restrictions on use: None
- 16. Distributor: See Below
- 17. Original source of software:

Developer: D.A. Calahan, Dept. of Elec. & Comp. Engineering Institution: University of Michigan, Ann Arbor, MI 48109; 313-763-0036 Sponsor: Air Force Office of Scientific Research

18. For further information contact: See Above

- 1. Name of program or package: SPAR/BL/CRAY
- 2. Descriptive title: General Block-Oriented Sparse Solver for CRAY-1
- 3. Problem domain: Unsymmetric matrices
- 4. Method of solution: LU factorization
- 5. Programming language: Fortran and CRAY Assembly Language
- 6. Precision: 64-bit

- 7. Portability: CRAY-1, CRAY-1S, CRAY X-MP
- 8. Other packages required:
- 9. Mode of use: Subroutine (s)
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 1800 Percentage comments: 20
- 12. Special features: Solves matrices blocked by row and column strips eminating from diagonal blocks.
- 13. Documentation and references:
 Detailed header comments?

User guide or manual, technical reports, papers, books:
"A Collection of Sparse Matrix Solvers for the CRAY-1", Report #166, Systems Engineering Laboratory, University of Michigan, Ann Arbor, MI 48109; October, 1982

- 14. Approximate cost of obtaining software: Send user tape
- 15. Restrictions on use: None
- 16. Distributor: See Below
- 17. Original source of software:

Developer: D.A. Calahan, Dept. of Elec. & Comp. Engineering Institution: University of Michigan, Ann Arbor, MI 48109

Sponsor: Air Force of Scientific Research

18. For further information contact: See Above

- 1. Name of program or package: SOLVEBLOK
- 2. Descriptive title: Direct almost block diagonal system solver
- 3. Problem domain: Almost block diagonal systems such as arise in spline approximation, e.g., in the pp collocation solution to ODE BVPs.
- 4. Method of solution: Gauss elimination with scaled partial pivoting
- 5. Programming language: Fortran V
- 6. Precision: single
- 7. Portability: developed on UNIVAC 1100, is running on various other machines
- 8. Other packages required: none
- 9. Mode of use: callable subroutine (s)
- 10. Test or demonstration program available? yes, part of package
- 11. Length of code in lines: 510

Percentage comments: (297/510) *100

- 12. Special features: none
- 13. Documentation and references:

Detailed header comments? yes

User guide or manual, technical reports, papers, books: ACM Trans. Math. Software 6(1980), 80-87; Algorithm 546, ACM Trans. Math. Software 6 (1980), 88-91.

- 14. Approximate cost of obtaining software: postage
- 15. Restrictions on use: none
- **16. Distributor:** ACM Algorithms Distribution service (listing), or send tape to developer (see 18.)
- 17. Original source of software:

Developer: C. de Boor & R. Weiss **Institution:** MRC, U.Wisconsin-Madison **Sponsor:**

18. For further information contact: C. de Boor, MRC, 610 Walnut St., Madison WI 53706

1. Name of program or package:

ARCECO

2. Descriptive title:

Almost block diagonal linear system solver

3. Problem domain:

Finite element methods for the solution of differential

equations in one space variable.

4. Method of solution:

Modified alternate row and column elimination

5. Programming language:

ANSI Fortran

6. Precision:

Double (changes for single indicated)

7. Portability:

IBM 370/165, IBM 3033/N8, DEC-10. Easily portable

8. Other packages required: None

9. Mode of use: Callable subroutine

10. Test or demonstration program available?

11. Length of code in lines:

1110

Percentage comments:

70%

12. Special features:

None

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

J.C. Diaz, G. Fairweather and P. Keast FORTRAN packages for solving almost block diagonal linear systems by modified alternate row and column elimination, Technical Report 148/81, Department of Computer Science, University of Toronto.

- 14. Approximate cost of obtaining software: Free on submission of a tape.
- 15. Restrictions on use:
- 16. Distributor:

Dr. P. Keast, Department of Computer Science, University of Toronto, Toronto, CANADA M5S 1A7

17. Original source of software:

Developer: J.C. Diaz, G. Fairweather, P. Keast

Institution: University of Kentucky and University of Toronto

Sponsor:

NSERC

18. For further information contact:

Dr. P. Keast, Department of Computer Science, University of Toronto, Toronto, CANADA M5S 1A7

1. Name of program or package:

ROWCOL

2. Descriptive title:

Almost block diagonal linear system solver

- 3. Problem domain: H⁻¹-Galerkin and collocation H⁻¹-Galerkin methods for
- differential equations in one space variable Method of solution:

Modified alternate row and column elimination

5. Programming language:

ANSI Fortran

- 6. Precision:
- Double (changes for single indicated) 7. Portability:

IBM 370/165, IBM 3033/N8, DEC-10. Easily portable.

- 8. Other packages required:
- 9. Mode of use:

Callable subroutine

10. Test or demonstration program available?

11. Length of code in lines:

Yes

Percentage comments:

74%

12. Special features:

None

13. Documentation and references:

Detailed header comments?

User guide or manual, technical reports, papers, books:

G. Fairweather and P. Keast, ROWCOL - a program for solving almost block diagonal linear systems arising in the H^{-1} -Galerkin and collocation H^{-1} -Galerkin methods, Technical Report, Department of Computer Science, University of Toronto, to appear.

- 14. Approximate cost of obtaining software: Free on submission of a tape.
- 15. Restrictions on use:
- 16. Distributor:

None

Dr. P. Keast, Department of Computer Science, University of Toronto, Toronto, Canada M5S 1A7

17. Original source of software:

Developer: G. Fairweather and P. Keast

Institution: University of Kentucky and University of Toronto

Sponsor:

NSERC

18. For further information contact:

Dr. P. Keast, Department of Computer Science, University of Toronto, Toronto, Canada M5S 1A7

- 1. Name of program or package: COLROW
- 2. Descriptive title:

Almost block diagonal linear system solver

- 3. Problem domain: Finite element methods for the solution of differential equations in one space variable.
- 4. Method of solution:

Modified alternate row and column elimination **5. Programming language:**

ANSI Fortran

- 6. Precision:
- Double (changes for single indicated) 7. Portability:

IBM 370/165, IBM 3033/N8, DEC-10. Easily portable.

8. Other packages required:

- 9. Mode of use:
- Callable subroutine
 10. Test or demonstration program available?
- 11. Length of code in lines: $_{1120}$

Percentage comments:

Yes

65%

12. Special features:

None

13. Documentation and references:

Detailed header comments?

User guide or manual, technical reports, papers, books:

J.C.Diaz, G. Fairweather, and P. Keast, FORTRAN packages for solving almost block diagonal linear systems by modified alternate row and column elimination, Technical Report 148/81, Department of Computer Science, University of Toronto.

- 14. Approximate cost of obtaining software: Free on submission of a tape.
- 15. Restrictions on use:
- 16. Distributor:

Dr. P. Keast, Department of Computer Science, University of Toronto, Toronto, CANADA M5S 1A7

17. Original source of software:

Developer: G. Fairweather and P. Keast

Institution: University of Kentucky and University of Toronto Sponsor:

NSERC

18. For further information contact:

Dr. P. Keast, Computer Science Department, University of Toronto. Toronto, Canada M5S 1A7

1. Name of program or package: MA27

2. Descriptive title: Solves linear sets of equations.

3. Problem domain: Sparse symmetric matrices, which need not be definite.

4. Method of solution: Symmetric factorization, including 2*2 pivots.

5. Programming language: IBM Fortran.

6. Precision: Both single and double precision versions are available.

7. Portability: Fortran 66 version available.

8. Other packages required: None.

9. Mode of use: Subroutine calls.

10. Test of demonstration program available: Yes.

11. Length of code in lines: 2922

Percentage comments: 37%

12. Special features: Multi-frontal approach, with vectorizable inner loops. Complex version (ME27)

13. Documentation and references:

Detailed header comments? Yes.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

I.S.Duff and J.K.Reid (1982), The multifrontal solution of indefinite sparse symmetric linear systems. To appear.

I.S.Duff and J.K.Reid (1982), MA27 – A set of Fortran subroutines for solving symmetric sets of linear equations. Harwell report R–10533, H.M.S.O., London.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (i), (ii), (iii), (iv) (see appendix on Harwell Subroutine Library).
- 16. Distributor: S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.

17. Original source of software:

Developer: I.S.Duff and J.K.Reid. **Institution:** A.E.R.E. Harwell. **Sponsor:** A.E.R.E. Harwell.

18. For further information contact: The developers.

1. Name of program or package: SPARSPAK

2. Descriptive title: Solution of Sparse Systems of Linear Equations

- 3. Problem domain: Systems of Equations having symmetric structure and for which no pivoting for stability is required; symmetric positive definite systems.
- 4. Method of solution:

Cholesky's method, Gaussian elimination

5. Programming language:

FORTRAN

6. Precision: SINGLE OR DOUBLE

7. Portability: Runs through PFORT; special IBM versions also available.

8. Other packages required: None

- 9. Mode of use: Sets of sub-routines callable from Fortran user program.
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines:

Percentage comments:

Approx. 20,000

Approx. 20%

12. Special features:

- friendly user interface
- easy to use SAVE and RESTART facility.

13. Documentation and references:

Detailed header comments? NO

User guide or manual, technical reports, papers, books:

- User Guide for SPARSPAK: Waterloo Sparse Linear Equations Package, Alan George, Joseph Liu, and Esmond Ng.
- Book: Computer Solution of Large Sparse Positive Definite Systems, Alan George and Joseph Liu, Prentice Hall, Inc., March 1981.
- 14. Approximate cost of obtaining software: US\$750.00 (one time charge for source code).
- 15. Restrictions on use: license agreement required
- 16. Distributor: Waterloo Research Institute

University of Waterloo

Waterloo, Ontario, CANADA N2L 3G1

17. Original source of software:

Developer: Alan George and Joseph Liu **Institution:** University of Waterloo

Sponsor: 1) Natural Sciences and Engineering Council of Canada

2)University of Waterloo

18. For further information contact:

Prof. Alan George Dept. of Computer Science University of Wacerloo

Waterloo, Ontario, CANADA N2L 3Gl.

1. Name of program or package: YSMP

2. Descriptive title: Yale Sparse Matrix Package

3. Problem domain: Re-ordering, Factorization and Solution of Symmetric and

nonsymmetric linear equations

4. Method of solution: Minimum degree ordering and Sparse Gaussian Elimination

5. Programming language: Fortran

6. Precision: Single (marked, simple conversion to double)

7. Portability: Developed on DEC-10, DEC-20, IBM/360, IBM/370, CDC-6600 Easily portable to other machines.

8. Other packages required: None

9. Mode of use: Callable subroutines (5 drivers + lower level subroutines)

10. Test or demonstration program available? γ_{es} (2)

11. Length of code in lines: 4000 Percentage comments: 59%

12. Special features: None

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

S. C. Eisenstat, M. C. Gursky, M. H. Schultz, and A. H. Sherman, Yale Sparse Matrix Package I: The Symmetric Codes, Int. J. Num. Mthds Engrg, to appear.

S. C. Eisenstat, M. C. Gursky, M. H. Schultz, and A. H. Sherman, Yale Sparse Matrix Package II: The Nonsymmetric Codes, Report 114, Dept. of Computer Science, Yale University, 1977.

14. Approximate cost of obtaining software: \$100.00

15. Restrictions on use: None

16. Distributor: YSMP Librarian

Department of Computer Science

Box 2158 Yale Station

17. Original sour of softwarenn. 06520

Developer:

Institution: Stanley C. Eisenstat, Martin H. Schultz, Andrew H. Sherman

Sponsor: Yale University

ONR, AFOSR

18. For further information contact:

Stanley C. Eisenstat Department of Computer Science Box 2158 Yale S⁺ +ion New Haven, CT 0:520

713/432-4674

1. Name of program or package: General Symmetric Sparse Solver (Symmetric SYMFAC, NUMFAC and BKSLVE)

2. Descriptive title: Symmetric sparse linear systems solver

3. Problem domain: Symmetric positive definite linear systems

4. Method of solution: SYMFAC - NUMFAC approach

5. Programming language: FORTRAN

6. Precision: Single and double precision

7. Portability: Standard FORTRAN

8. Other packages required: None

9. Mode of use: Callable FORTRAN subroutines

10. Test or demonstration program available? Yes

11. Length of code in lines: about 500 Percentage comments: about 50%

12. Special features:

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

Some Results on Sparse Matrices, IBM Research Report 1980 "Some Basic Techniques for Solving Sparse Systems of Linear Equations," Sparse Matrices and their Applications, D. J. Rose and R. A. Willoughby (eds.) Plenum Press, 1972, pp. 41-52

- 14. Approximate cost of obtaining software: See 18.
- 15. Restrictions on use: None
- 16. Distributor: Same as 18.

17. Original source of software:

Developer: Fred G. Gustavson IBM Research **Sponsor:**

18. For further information contact:

Dr. Fred G. Gustavson 33-205 IBM T. J. Watson Research Center P.O. Box 218 Yorktown Heights, New York 10598 Phone: (914) 945-1980

- 1. Name of program or package: RSFS
- 2. Descriptive title: Sparse linear system solver
- 3. Problem domain: Real, symmetric linear systems
- 4. Method of solution: LDU Decomposition
- 5. Programming language: FPS-164 Array Processor
- 6. Precision: 64-bit word
- 7. Portability: Developed for the FPS-164 Array Processor. A version also exists for the following FPS 38-bit Array Processors:
- 8. Other packages required: FPS-100, AP-120B, AP-180V, and AP-190L. FPS-164 Math Library (APMATH64)
 9. Mode of use: Callable subroutine
- 10. Test or demonstration program available? $_{
 m NO}$
- 11. Length of code in lines: 1112

Percentage comments:70

- 12. Special features: Takes advantage of the parallel, pipelined architecture of the FPS-164 Array Processor.
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

APMATH64 Reference Manual Floating Point Systems, Inc.

- 14. Approximate cost of obtaining software: This routine is included in the
- FPS-164 Math Library (APMATH64).

 15. Restrictions on use: License agreement required
- 16. Distributor: Floating Point Systems, Inc.

P.O. Box 23489

Portland, Or. 97223

(503) 641-3151 17. Original source of software:

Developer: Ron Coleman Institution: Floating Point Systems, Inc.

Sponsor: Floating Point Systems, Inc.

18. For further information contact:

Phil Vaughn

Floating Point Systems, Inc

P.O. Box 23489

Portland, OR 97223

(503) 641-3151 TLX: 360470 FLOATPOIN BEAV

- 1. Name of program or package: CSPARSPAK
- 2. Descriptive title: Complex version of sparse linear system solver, SPARSPAK.
- 3. Problem domain: Large sparse complex systems of linear equations; most efficient for symmetric or Hermitian matrices.
- 4. Method of solution: Choice of 5 reordering algorithms followed by sparse Gaussian elimination.
- 5. Programming language: FORTRAN
- 6. Precision: Single
- 7. Portability: Developed on CYBER, IBM; portable.
- 8. Other packages required: SPARSPAK
- 9. Mode of use: Collection of subroutines.
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 9000 lines Percentage comments: about 50%
- 12. Special features: User insulated from complicated data structures and storage management.
- 13. Documentation and references: Detailed header comments? Yes User guide or manual, technical reports, papers, books: SPARSPAK User Guide
- 14. Approximate cost of obtaining software: CSPARSPAK is available to BCS network users.
- Possibility of sale to interested organizations is under review.

 15. Restrictions on use:
 Use on BCS systems or if sold, internal use only. May not be distributed to others.

 16. Distributor: Boeing Computer Services Company
- 17. Original source of software:

Developer: J.G. Lewis modified SPARSPAK (developed by Alan George & Joseph Liu).

Institution: Boeing Computer Services Company Boeing Computer Services Company

18. For further information contact: J.G. Lewis

Boeing Computer Services Company 565 Andover Park West, MS 9C-01 Tukwila, WA 98188

(206) 575-5102

- 1. Name of program or package: CSFS
- 2. Descriptive title: Sparse linear system solver
- 3. Problem domain: Complex, symmetric linear systems
- 4. Method of solution: LDU Decomposition
- 5. Programming language: Assembly language FPS-164 Array Processor
- 6. Precision: 64-bit word

- 7. Portability: Developed for the FPS-164 Array Processor. A version also exists for the following FPS 38-bit Array Processors:
- FPS-100, AP-120B, AP-180V, and AP-190L.

 8. Other packages required: FPS-164 Math Library (APMATH64)
- 9. Mode of use: Callable subroutine
- 10. Test or demonstration program available? N_{O}
- 11. Length of code in lines: 1421 Percentage comments: 71
- 12. Special features: Takes advantage of the parallel, pipelined architecture of of the FPS-164 Array Processor.
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

APMATH64 Reference Manual Floating Point Systems, Inc.

- 14. Approximate cost of obtaining software: This routine is included in the FPS-164 Math Library (APMATH64).
- 15. Restrictions on use: License agreement required.
- 16. Distributor: Floating Point Systems, Inc.

P.O. Box 23489

(503) 641-3151 Portland, OR 97223

17. Original source of software:

Developer: Ron Coleman

Institution: Floating Point Systems, Inc. Floating Point Systems, Inc. Sponsor:

18. For further information contact:

Phil Vaughn

Floating Point Systems, Inc.

P.O. Box 23489

Portland, OR 97223

(503) 641-3151 TLX: 360470 FLOATPOIN BEAV

1. Name of program or package: F01MCF

2. Descriptive title: Factorises a matrix

3. Problem domain: Symmetric, positive definite, variable bandwidth matrix

4. Method of solution: Cholesky

5. Programming language: FORTRAN

6. Precision: Either

7. Portability: Available on 48 machine ranges/compilers

8. Other packages required: NAG

9. Mode of use: Callable subroutine

10. Test or demonstration program available? Yes

11. Length of code in lines: 126 Percentage comments: 54%

12. Special features:

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

NAG Library Manual NAG On-line Supplement

- 14. Approximate cost of obtaining software: NAG Library costs \$1584/year
- 15. Restrictions on use: License agreement
- **16. Distributor:** NAG (U.S.A.) Inc. (see below)
- 17. Original source of software:

Developer: Dr. M. Cox Institution: N.P.L.
Sponsor: NAG

18. For further information contact:

Mrs. Carolyn M. Smith
NAG (U.S.A.) Inc.
1250 Grace Court
Downers Grove, IL 60516
Tel. 971-2337
Telex 23254708 (Telesery DFLD)

1. Name of program or package: F04MCF

2. Descriptive title: Solves a system of linear algebraic equations

3. Problem domain: Symmetric, positive-definite variable bandwidth matrix

4. Method of solution: Cholesky

5. Programming language: FORTRAN

6. Precision: Either

7. Portability: Available on 48 machine ranges/compilers

8. Other packages required: NAG

9. Mode of use: Callable subroutine

10. Test or demonstration program available? Yes

11. Length of code in lines: 155 Percentage comments: 76%

12. Special features:

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

NAG Library Manual NAG On-line Supplement

- 14. Approximate cost of obtaining software: NAG Library License costs \$1584/year
- 15. Restrictions on use: License agreement
- 16. Distributor: NAG (U.S.A.) Inc. (see below)
- 17. Original source of software:

Developer: Dr. M. Cox Institution: N.P.L. Sponsor: NAG

18. For further information contact:

Mrs. Carolyn M. Smith
NAG (U.S.A.) Inc.
1250 Grace Court
Downers Grove, IL 60516
Tel. 971-2337
Telex 23254708 (Telexerv DFLD)

1. Name of program or package: MA15

2. Descriptive title: Solve linear sets of equations.

3. Problem domain: Symmetric positive-definite banded matrices.

4. Method of solution: Symmetric factorization.

5. Programming language: IBM Fortran.

6. Precision: Both single and double precision versions are available.

7. Portability: Fortran 77 version available.

8. Other packages required: Harwell subroutine FM01.

9. Mode of use: Subroutine calls.

10. Test of demonstration program available: Yes.

11. Length of code in lines: 147 Percentage comments: 4%

(252 with dependencies)

12. Special features: Overflows to direct-access file if necessary.

13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

J.K.Reid (1972), Two Fortran subroutines for direct solution of linear equation whose matrix is sparse, symmetric and positive definite. Harwell report R.7119, H.M.S.O., London.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii), (iii) (see appendix on Harwell Subroutine Library).
- 16. Distributor: S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.

17. Original source of software:

Developer: J.K.Reid.

Institution: A.E.R.E. Harwell. Sponsor: A.E.R.E. Harwell.

18. For further information contact: The developer.

- 1. Name of program or package: PROFILE/S/CRAY
- 2. Descriptive title: Symmetric Banded and Profile Solvers for the CRAY-1
- 3. Problem domain: Symmetric banded and profile matrices
- 4. Method of solution: U^TDU factorization
- 5. Programming language: CRAY assembly language
- 6. Precision: 64-bit
- 7. Portability: CRAY-1, CRAY-1S, CRAY X-MP
- 8. Other packages required: None
- 9. Mode of use: Subroutine
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 2500 Percentage comments: 20
- 12. Special features: Compressed storage by rows or columns; no bandwidth restriction; achieves 120 MFLOPS with bandwidth greater than 40.
- 13. Documentation and references: Detailed header comments? $$^{\rm NO}$$

User guide or manual, technical reports, papers, books:

"High Performance Banded and Profile Solvers for the CRAY-1: The Symmetric Case" Report #165, Systems Engineering Laboratory, University of Michigan, Ann Arbor, MI 48109; August 1982.

- 14. Approximate cost of obtaining software: Send user tape
- 15. Restrictions on use: None
- 16. Distributor: See Below
- 17. Original source of software:

Developer: D.A. Calahan, Dept. of Elec. & Comp. Engineering Institution: University of Michigan, Ann Arbor, MI 48109; 313-763-0036 Sponsor: Air Force Office of Scientific Research

18. For further information contact: See Above

- 1. Name of program or package: SKYSOL
- 2. Descriptive title: Sparse linear system solver
- 3. Problem domain: Real, symmetric, skyline profile linear systems
- 4. Method of solution: LU Decomposition
- 5. Programming language: Assembly Language FPS-164 Array Processor
- 6. Precision: 64-bit word
- 7. Portability: Developed for the FPS-164 Array Processor. A version also exists for the following FPS 38-bit Array Processors: FPS-100, AP-120B, AP-180V, and AP-190L.

 8. Other packages required: FPS-164 Math Library (APMATH64)
- 9. Mode of use: Callable subroutine
- 10. Test or demonstration program available? No
- 11. Length of code in lines: 576

Percentage comments: 50

- 12. Special features: Takes advantage of the parallel, pipelined architecture of the FPS-164 Array Processor.
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

APMATH64 Reference Manual Floating Point Systems, Inc.

- 14. Approximate cost of obtaining software: This routine is included in
- the FPS-164 Math Library (APMATH64).

 15. Restrictions on use: License agreement required
- 16. Distributor: Floating Point Systems, Inc.

P.O. Box 23489

Portland, OR 97223

17. Original source of software:

Developer: L. Tarvestad

Institution: Floating Point Systems, Inc. Sponsor: Floating Point Systems, Inc.

18. For further information contact:

Phil Vaughn Floating Point Systems, Inc. P.O. Box 23489

Portland, OR 97223

(503) 641-3151 TLX: 360470 FLOATPOIN BEAV

- 1. Name of program or package: ITPACK 2C
- 2. Descriptive title: Sparse linear system solver using iterative methods
- 3. Problem domain: The seven ITPACK routines can be called with any linear system con-

taining positive diagonal elements, however they are most successful in solving systems with symmetric positive definite or mildly nonsymmetric matrices.

4. Method of solution: Jacobi Conjugate Gradient, Jacobi Semi-iteration, SOR, Symmetric SOR Conjugate Gradient, Symmetric SOR semi-iteration, Reduced System Conjugate Gradient, Reduced System Semi-iteration

5. Programming language:

ANSI FORTRAN 66

6. Precision: Single

- 7. Portability: Easily portable since entire package written in ANSI FORTRAN 66. Was developed on a CDC CYBER 170/750 but tested on other computers.
- 8. Other packages required: None
- 9. Mode of use: Callable subroutines
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 8960 Percentage comments: 51%
- 12. Special features: Uses sparse storage scheme (symmetric or nonsymmetric). Automatic selection of the acceleration parameters and the use of accurate stopping criteria are major features of this software package.
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

"ITPACK 2C: A Fortran Package for Solving Large Sparse Linear Systems by Adaptive Accelerated Iterative Methods", David R. Kincaid, John R. Respess, David M. Young, and Roger G. Grimes, ACM Transactions on Mathematical Software, Vol. 8, No. 3, September 1982.

Applied Iterative Methods, Louis A. Hageman and David M. Young, Academic Press,

- 14. Approximate cost of obtaining software: Mag. Tape \$76.50 ACM Member; \$90 Others
- 15. Restrictions on use: None
- ACM ALGORITHMS DISTRIBUTION SERVICE 16. Distributor: International Mathematical and Statistical Libraries, Inc. Sixth Floor, NBC Building, 7500 Bellaire Boulevard Houston, Texas 77036 (713) 772-1927 Houston, Texas 77036
- 17. Original source of software:

Developer: David R. Kincaid, Roger G. Grimes, John R. Respess, David M. Young Institution: Center for Numerical Analysis, University of Texas at Austin

Sponsor: National Science Foundation

18. For further information contact: John R. Respess, Center for Numerical Analysis

University of Texas at Austin RLM 13.150

Austin, Texas 78712 (512) 471-1242

ARPANET: RESPESS@UTEXAS-11

- 1. Name of program or package: SITSOL
- 2. Descriptive title: Sparse linear system solver
- 3. Problem domain: Real, unsymmetric linear systems
- 4. Method of solution: SOR or Gauss-Seidel
- 5. Programming language: Assembly language FPS-164 Array Processor
- 6. Precision: 64-bit word

- 7. Portability: Developed for the FPS-164 Array Processor.
- 8. Other packages required: FPS-164 Math Library (APMATH64)
- 9. Mode of use: Callable subroutine
- 10. Test or demonstration program available? N_{O}
- 11. Length of code in lines: 742

Percentage comments:77

- **12. Special features:** Takes advantage of the parallel, pipelined architecture of the FPS-164 array processor.
- 13. Documentation and references:
 Detailed header comments? Yes
 User guide or manual, technical reports, papers, books:
 APMATH64 Reference Manual
 Floating Point Systems, Inc.
- 14. Approximate cost of obtaining software: This routine is included in the FPS-164
- Math Library (APMATH64)

 15. Restrictions on use: License agreement required
- **16. Distributor:** Floating Point Systems, Inc. P.O. Box 23489

Portland, OR 97223

17. Original source of software:

Developer: Ron Coleman

Institution: Floating Point Systems, Inc.
Sponsor: Floating Point Systems, Inc.

18. For further information contact:

Phil Vaugh
Floating Point Systems, Inc.
P.O. Box 23489
Portland, OR 97223
(503) 641-3151 TLX: 360470 FLOATPOIN BEAV

1. Name of program or package: TCHLIB

2. Descriptive title: Sparse Linear System Solver

3. Problem domain: Symmetric and Nonsymmetric Linear Systems

4. Method of solution: Tchebychev iteration with Dynamic Estimation of Parameters

5. Programming language: FORTRAN

6. Precision: Single

7. Portability: Passes PFORT Verifier

8. Other packages required: BLAS, EISPACK

9. Mode of use: Subroutine

10. Test or demonstration program available? Yes

11. Length of code in lines: 2734 Percentage comments: 40%

12. Special features: Highly vectorized

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books: None

14. Approximate cost of obtaining software: None

15. Restrictions on use: None

16. Distributor: NESC

17. Original source of software:

Developer: T. A. Manteuffel

Institution: Los Alamos National Laboratory

Sponsor: DOE

18. For further information contact:

T. A. Manteuffel Mail Stop B265 Los Alamos National Laboratory Los Alamos, NM 87545 1. Name of program or package:

2. Descriptive title: Sparse linear system solver

Symmetric systems, definite or indefinite 3. Problem domain:

4. Method of solution: Lanczos tridiagonalization

5. Programming language: ANSI FORTRAN

6. Precision: Single, easily converted to double

Developed on IBM and Burroughs; easily portable to other machines 7. Portability:

8. Other packages required: BLAS if available; simplified alternatives provided

9. Mode of use: Callable subroutine

10. Test or demonstration program available? Yes

11. Length of code in lines: 500 60% Percentage comments:

12. Special features: BLAS operations are efficient in a paging

> environment and on pipeline machines. Overall efficiency may depend on user's own

routine for computing matrix-vector products y = Ax.

13. Documentation and references: **Detailed header comments?** Yes

User guide or manual, technical reports, papers, books:

Paper: C.C. Paige and M.A. Saunders, "Solution of sparse indefinite systems of linear equations", SIAM Journal of Numerical Analysis,

Vol. 12, No. 4, September 1975, 617-629.

14. Approximate cost of obtaining software: Zero, if tape is returned after use.

15. Restrictions on use:

None

16. Distributor:

Michael Saunders

Ph: (415)497-1875

Department of Operations Research

Stanford University, Stanford, CA 94305

17. Original source of software:

Developer: Institution: Chris Paige

Michael Saunders

McGill University Sponsor: National Research Council of Canada; DSIR, New Zealand;

Stanford University

AEC. NSF.

18. For further information contact:

Michael Saunders (see 16 above)

- 1. Name of program or package: ICCG-package
- 2. Descriptive title: Mathematical software for elliptic boundary value problems.
- Problem domain: Self-adjoint/mixed, periodic boundary conditions/2 D rectangular domains.
- 4. Method of solution: Standard finite differences with conjugate gradient iteration technique, preconditioned with imcomplete Choleski factorization.
- 5. Programming language: FORTRAN (ANSI)
- 6. Precision: Single

- 7. Portability: Portable FORTRAN (PFORT verifier); tested on Cyber 175-28 (CDC)
- 8. Other packages required: None
- 9. Mode of use: Callable subroutines
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: ca. 3000 Percentage comments: over 50%
- 12. Special features:

Versions for space or time economization

13. Documentation and references: Available Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

- J. M. van Kats & H. A. van der Vorst, "Software for the discretisation and solution of second order self-adjoint elliptic partial differential equations in two dimensions,: TR-10, ACCU, Budapestlaan 6, Utrecht, The Netherlands
- 14. Approximate cost of obtaining software: Free
- 15. Restrictions on use: Notes
- 16. Distributor: ACCU, Budapestlaan 6, Utrecht, The Netherlands
- 17. Original source of software: A.C.C.U.

Developer: Jan van Kats & Henk van der Vorst Institution: Academic Computer Centre Utrecht Sponsor: Utrecht University

18. For further information contact:

Henk van der Vorst ACCU Budapestlaan 6 Utrecht The Netherlands

- 1. Name of program or package: MA31
- 2. Descriptive title: Solves linear sets of equations.
- 3. Problem domain: Symmetric sparse positive-definite matrices.
- 4. Method of solution: Incomplete factorization and conjugate gradients.
- 5. Programming language: IBM Fortran.
- 6. Precision: Both single and double precision versions are available.
- 7. Portability: Fortran 66 version available.
- 8. Other packages required: None.
- 9. Mode of use: Subroutine calls.
- 10. Test of demonstration program available: Yes.
- 11. Length of code in lines: 1111

Percentage comments: 35%

- 12. Special features: Contains a parameter to adjust the amount of fill. It can therefore be used as a direct solver with iterative refinement or as an iterative solver requiring a variable amount of storage.
- 13. Documentation and references:

Detailed header comments? Yes.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

N. Munksgaard (1980) Solving sparse symmetric sets of linear equations by preconditioned conjugate gradients. A.C.M. Trans. Math. Software, 6, 206–219.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii), (iii) (see appendix on Harwell Subroutine Library).
- 16. Distributor: S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.
- 17. Original source of software:

Developer: N.Munksgaard.

Institution: Technical University of Denmark.

Sponsor: Danish Natural Science Research Council.

18. For further information contact: I.S.Duff or J.K.Reid at Harwell.

1. Name of program or package:

PCGPAK

2. Descriptive title:

Sparse linear system solver.

3. Problem domain:

General nonsingular sparse linear systems.

4. Method of solution:

Preconditioned conjugate gradient method and conjugate gradient-like

5. Programming language:

FORTRAN

6. Precision:

Either 7. Portability:

Developed on DEC-20 and VAX-780. Easily portable.

8. Other packages required:

9. Mode of use:

BLAS

Callable subroutine.

10. Test or demonstration program available?

11. Length of code in lines:

Percentage comments:

length 2700

percentage 30%

12. Special features:

None

13. Documentation and references:

Detailed header comments?

User guide or manual, technical reports, papers, books:

S. C. Eisenstat, H. C. Elman, M. H. Schultz.

Variational iterative methods for nonsymmetric systems of linear equations. Technical Report #209, Yale University, Dept. of Computer Science, 1981.

14. Approximate cost of obtaining software:

15. Restrictions on use:

Software not available for distribution at present.

16. Distributor:

17. Original source of software: Howard C. Elman, Stanley C. Eisenstat, Martin H. Schultz Developer:

Institution: Yale University, Dept. of Computer Science
Sponsor: ONR, NSF, Scientific Computing Associates

18. For further information contact:

Howard C. Elman Yale Univ. Dept. of Computer Science P.O. Box 2158 Yale Station New Haven, CT 06520

(203) 432-4674

- 1. Name of program or package: CG25, BCG25, CCG25.
- Descriptive title: Packages for solving five diagonal systems of algebraic equations.
- 3. Problem domain: Solves systems of five diagonal systems of equations such as arise in finite difference models of two dimensional elliptic partial differential equations. CG is for symmetric systems, BCG for unsymmetric systems and CCG for 4. Method of solution:

 Preconditioned Conjugate Gradients.
- 5. Programming language: ANSI FORTRAN 66.
- 6. Precision: Single and double precision versions available.
- 7. Portability: Developed on IBM, but written in ANSI FORTRAN.
- 8. Other packages required: None
- 9. Mode of use: Callable subroutine.
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: About 2000 each Percentage comments: About 70%
- **12. Special features:** Written for computational efficiency and for ease of modification and further enhancement. Hence the development of specialized versions for very large problems, for example, which use particular features of a computer, is made as easy as possible.
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

Program Note RD/L/2234 P81: CG25, BCG25, CCG25: Packages for solving five diagonal systems of algebraic equations using preconditioned conjugate gradient methods. Author: D.A.H. Jacobs, Central Electricity Research Laboratories, Leatherhead, Surrey, England.

- 14. Approximate cost of obtaining software: On application
- 15. Restrictions on use: License Agreement Required
- **16. Distributor:** External Sales, Headquarters Computing Centre, Central Electricity Generating Board, 85 Park Street, London, SEl 9DY, England, Tele. Ol 248 1202.
- 17. Original source of software:

Developer: D.A.H. Jacobs

Institution: Central Electricity Research Labs., Leatherhead, Surrey, England.

Sponsor: Central Electricity Generating Board

18. For further information contact: For sales: Mr. M. Wall (address in 16 above)

Technical Queries: Dr. D.A.H. Jacobs, Central Electricity Research Labs.,

Kelvin Avenue, Leatherhead, Surrey, England,

Tele. 0372 374488

- 1. Name of program or package: CG37, BCG37, CCG37.
- 2. Descriptive title: Packages for solving seven diagonal systems of algebraic equations.
- 3. Problem domain: Solves systems of seven diagonal systems of equations such as arise in finite difference models of three dimensional elliptic partial differential equations. CG is for symmetric systems, BCG for unsymmetric systems and CCG for 4. Method of solution:

 complex systems

Preconditioned Conjugate Gradients

- 5. Programming language: ANSI FORTRAN 66
- 6. Precision: Single and double precision versions available.
- 7. Portability: Developed on IBM, but written in ANSI FORTRAN.
- 8. Other packages required: None

- 9. Mode of use: Callable subroutine
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: About 2000 each Percentage comments: About 70%
- **12. Special features:** Written for computational efficiency and for ease of modification and further enhancement. Hence the development of specialized versions for very large problems, for example which use particular features of a computer, is made as easy as possible.
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

Program Note RD/L/2235 P81: CG37, BCG37, CCG37: Packages for solving seven diagonal systems of algebraic equations using preconditioned conjugate gradient methods. Author: D.A.H. Jacobs, Central Electricity Research Laboratories, Leatherhead, Surrey, England.

- 14. Approximate cost of obtaining software: On application
- 15. Restrictions on use: License agreement required
- 16. Distributor: External Sales, Headquarters Computing Centre, Central Electricity Generating Board, 85 Park Street, London, SEI 9DY, England, Tele. 01 248 1202.
- 17. Original source of software:

Developer: D.A.H. Jacobs

Institution: Central Electricity Research Labs., Leatherhead, Surrey, England

Sponsor: Central Electricity Generating Board

18. For further information contact: For sales: Mr. M. Wall (address in 16 above)

Technical Queries: Dr. D.A.H. Jacobs, Central Electricity Research Labs.,

Kelvin Avenue, Leatherhead, Surrey, England,

Tele. 0372 374488

- 1. Name of program or package: CGS, BCGS, CCGS
- 2. Descriptive title: Sparse code packages for solving general irregular systems of algebraic equations.
- 3. Problem domain: Solves systems of equations whose matrices are irregular (i.e. non-banded) such as arise for example from finite element formulations of elliptic partial differential equations. CGS is for symmetric systems. BCGS for unsymmetric 4. Method of solution:

 systems, and CCGS for general complex systems

Precondtioned Conjugate Gradients

- 5. Programming language: ANSI FORTRAN 66
- **6. Precision:** Single and double precision versions available
- 7. Portability: Developed on IBM but written in ANSI FORTRAN
- 8. Other packages required: None
- 9. Mode of use: Callable subroutine
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: Percentage comments: Approx. 75% CGS approx 1500, BCGS/CCGS approx 2000
- 12. Special features: Written for computational efficiency and for ease of modification and further enhancement (modular approach, fully internally documented).
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

Program Note to be published, A user's guide to CGS, BCGS and CCGS: sparse code packages using precodnitioned conjugate gradient methods for solving systems of algebraic equations. Author: G. Markham

- 14. Approximate cost of obtaining software: On application
- 15. Restrictions on use: License agreement required
- 16. Distributor: External Sales, Headquarters Computing Centre, Central Electricity Generating Board, 85 Park Street, London, SEI 9DY, England. Tele 01 248 1202
- 17. Original source of software:

Developer: G. Ma:

Institution: Central Electricity Research Laboratories
Sponsor: Central Electricity Generating Board

18. For further information contact: Sales: (Mr. M. Wall (address as for 16 above)

Technical queries: G. Markham, Central Electricity Research Laboratories

Kelvin Avenue, Leatherhead, Surrey, England, KT22 7SE.

Tele: 0372 374488

- 1. Name of program or package: DI205, DI3707, DI209, DI213
- 2. Descriptive title: Subroutines to solve a five, seven, nine and thirteen diagonal system of algebraic equations.
- 3. Problem domain: Solves systems of multi-diagonal systems of equations such as arise in finite difference models of partial differential equations. Five, nine and thirtgen point molecules in two dimensions, and seven point in three dimensions can be used. Extensions to cover small perturbations on these structures can be employed.
- 4. Method of solution: Stone's Strongly Implicit Procedure
- 5. Programming language: ANSI FORTRAN 66
- 6. Precision: Single and double precision versions available.
- 7. Portability: Developed on IBM, but written in ANSI FORTRAN.
- 8. Other packages required: None
- 9. Mode of use: Callable subroutine
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: About 2000 each Percentage comments: About 70%
- 12. Special features: Written for computational efficiency and for ease of modification and further enhancement. Hence the development of specialized versions for very large problems, for example which use particular features of a computer, is made as easy as possible.
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

Program Notes: RD/L/P9/79: DI205; RD/L/P11/79: DI307; RD/L/P14/79: DI209; RD/L/P18/79: DI213. Author: D.A.H. Jacobs, Central Electricity Research Laboratories, Leatherhead, Surrey, England

- 14. Approximate cost of obtaining software: On application
- 15. Restrictions on use: License agreement required
- **16. Distributor:** External Sales, Headquarters Computing Centre, Central Electricity Generating Board, 85 Park Street, London, SEl 9DY, England, Tele. Ol 248 1202.
- 17. Original source of software:

Developer: D.A.H. Jacobs

Institution: Central Electricity research Labs., Leatherhead, Surrey, England

Sponsor: Central Electricity Generating Board

18. For further information contact: For sales: Mr. M. Wall (address in 16 above) Technical Queries: Dr. D.A.H. Jacobs, Central Electricity Research Labs., Kelvin Avenue, Leatherhead, Surrey, England, Tele. 0372 374488.

1. Name of program or package: D03EBF

2. Descriptive title: Solver for Systems of Simultaneous Algebraic Equations

3. Problem domain: Equations of five-point Molecule form on a two dimensional

topologically rectangular mesh

4. Method of solution: Strongly Implicit Procedure

5. Programming language: FORTRAN

6. Precision: Either

7. Portability: Available on 48 machine ranges/compliers

8. Other packages required: NAG

9. Mode of use: Callable subroutine

10. Test or demonstration program available? Yes

11. Length of code in lines: 297 Percentage comments: 66%

12. Special features:

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

NAG Library Manual NAG Library On-line Supplement

14. Approximate cost of obtaining software: NAG Library costs \$1584/year

15. Restrictions on use: License agreement

16. Distributor: NAG (U.S.A.) Inc., 1250 Grace Court, Downers Grove, IL 60516

Tel. 971-2337

17. Original source of software:

Developer: Dr. D. Jacobs **Institution:** C.E.G.B. (U.K.)

Sponsor: NAG

18. For further information contact:

Mrs. Carolyn M. Smith NAG (U.S.A.) Inc. 1250 Grace Court Downers Grove, IL 60516 Tel. 971-2337 Telex 23254708 (Teleserv DFLD) 1. Name of program or package: D03ECF

2. Descriptive title: Solver for Systems of Simultaneous Algebraic Equations

3. Problem domain: Equations of seven-point molecule form on a topologically

rectangular mesh.

4. Method of solution: Strongly Implicit Procedure

5. Programming language: FORTRAN

6. Precision: Either

7. Portability: Available on 48 machine ranges/compliers

8. Other packages required: NAG

9. Mode of use: Callable subroutine

10. Test or demonstration program available? YES

11. Length of code in lines: 358 Percentage comments: 70%

12. Special features:

13. Documentation and references:
Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

NAG Library Manual NAG Library On-line Supplement

- 14. Approximate cost of obtaining software: NAG Library costs \$1584/year
- 15. Restrictions on use: License agreement

16. Distributor: NAG (U.S.A.) Inc. (see below)

17. Original source of software:

Developer: Dr. D. Jacobs Institution: C.E.G.B. NAG

18. For further information contact:

Mrs. Carolyn M. Smith
NAG (U.S.A.) Inc.
1250 Grace Court
Downers Grove, IL 60516
Tel. 971-2337
Telex 23254708 (Telesery DFLD)

1. Name of program or package: D03UAF

2. Descriptive title: Performs one iteration of the Strongly Implicit Procedure.

3. Problem domain: Algebraic equations of five-point molecule form on a topologically rectangular mesh.

4. Method of solution: Strongly Implicit Procedure

5. Programming language: FORTRAN

6. Precision: Either

7. Portability: Available on 48 machine ranges/compilers

8. Other packages required: NAG

9. Mode of use: Callable Subroutine

10. Test or demonstration program available? Yes

11. Length of code in lines: 375 Percentage comments: 66%

12. Special features:

13. Documentation and references:

Detailed header comments?

Yes

User guide or manual, technical reports, papers, books:

NAG Library Manual NAG On-line Supplement

14. Approximate cost of obtaining software: NAG Library costs \$1584/year

15. Restrictions on use: License agreement

16. Distributor: NAG (U.S.A.) Inc. (see below)

17. Original source of software:

Developer: Dr. D. Jacobs Institution: C.E.G.B.
Sponsor: NAG

18. For further information contact:

Mrs. Carolyn M. Smith
NAG (U.S.A.) Inc.
1250 Grace Court
Downers Grove, IL 60516
Tel. 971-2337
Telex 23254708 (Teleserv DFLD)

1. Name of program or package: D03UBF

2. Descriptive title: Performs one iteration of the Strongly Implicit Procedure

3. Problem domain: Algebraic Equations of seven-point molecule form on a topologically rectangular mesh.

4. Method of solution: Strongly Implicit Procedure

5. Programming language: Fortran

6. Precision: Either

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7. Portability: Available on 48 machine ranges/compilers

8. Other packages required: NAG

9. Mode of use: Callable subroutine

10. Test or demonstration program available? Yes

11. Length of code in lines: 468 Percentage comments: 50%

12. Special features:

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

NAG Library Manual NAG On-line Supplement

- 14. Approximate cost of obtaining software: NAG Library costs \$1584/year
- 15. Restrictions on use: License agreement

16. Distributor: NAG (U.S.A.) Inc.

17. Original source of software:

Developer: Dr. D. Jacobs Institution: C.E.G.B. NAG

18. For further information contact:

Mrs. Carolyn M. Smith
NAG (U.S.A.) Inc.
1250 Grace Court
Downers Grove, IL 60516
Tel. 971-2337
Telex 23254708 (Telesery DFLD)

- 1. Name of program or package: LLSS01
- 2. Descriptive title: Sparse linear least squares and linear system package
- 3. Problem domain: Linear least squares and unsymmetric linear systems
- 4. Method of solution: Orthogonalization
- 5. Programming language: IBM Fortran H
- 6. Precision: Mixed7. Portability: Portable
- 8. Other packages required: None
- 9. Mode of use: Callable subroutines
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: about 1000 Percentage comments: 10%
- 12. Special features: None

13. Documentation and references:

Detailed header comments? No

User guide or manual, technical reports, papers, books:

Two technical reports at the Numerical Institute, Technical University of Denmark, Lyngby, Denmark;

Comp. & Maths.with Appls., 8(1982), pp. 119-135

- 14. Approximate cost of obtaining software: Free of charge
- 15. Restrictions on use: None
- **16. Distributor:** Numerical Institute, Technical University of Denmark, Lyngby, Denmark

17. Original source of software:

Developer: Z.Zlatev and H.B.Nielsen
Institution: Numerical Institute, Technical University of Denmark
Sponsor: The Danish Technical Science Research Council

18. For further information contact: H. B. Nielsen, Numerical Institute,

Technical University of Denmark

Lyngby, Denmark

1. Name of program or package: SPARSPAK - B

2. Descriptive title: Sparse matrix package

3. Problem domain: General square systems of linear equations, least squares problems, underdetermined systems of linear equations.

4. Method of solution: Orthogonal decomposition

5. Programming language: FORTRAN

6. Precision: Either single or double

7. Portability: Developed on IBM4341 using ANSI FORTRAN.

8. Other packages required: SPARSPAK

9. Mode of use: Callable subroutines

10. Test or demonstration program available? Yes

11. Length of code in lines: 9000 Percentage comments: about 10%

12. Special features: Require use of secondary storage

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books: User guide is available

14. Approximate cost of obtaining software: \$100.00 distribution fee

15. Restrictions on use: none

16. Distributor: Waterloo Research Institute

Needles Hall

University of Waterloo, Waterloo, Ontario, CANADA, N2L 3G1.

17. Original source of software:

Developer:

Alan George, Michael Heath, Esmond Ng

institution:

University of Waterloo

Sponsor:

Natural Sciences and Engineering Research Council of Canada

and U.S. Department of Energy

18. For further information contact:

Dr. Alan George Department of Computer Science University of Waterloo Waterloo, Ontario CANADA N2L 3G1

Phone: (519) 885-1211, ext.3473

- 1. Name of program or package: LASSO
- 2. Descriptive title: Least square Adjustments for Sparse Systems, Out-of-core with optional inverse elements.
- 3. Problem domain: Symmetric positive definite linear systems with reordering of equations to minimize storage. Primarily least square adjustments.
- 4. Method of solution: Minimum column profile reordering and Cholesky factorization.
- 5. Programming language: FORTRAN (compatible with FORTRAN 77)
- 6. Precision: Double precision.

- 7. Portability: Operational on Univac 1100, IBM 360/195, IBM 3300. Portability depends on FORTRAN 77, and logical functions for AND, OR, and LOCF the memory location of an array.

 8. Other packages required: Optional interface for SPARSPAK, but not required
- 9. Mode of use: Subroutine calls.
- 10. Test or demonstration program available? Yes
- Percentage comments: 5-10% 11. Length of code in lines: 7000
- 12. Special features: Input is usually observation equations and output is solution vector and optional partial matrix inverse (ie. elements inside sparse storage).

Optional assembly code for disk I/O on Univac 1100 and IBM 360.

13. Documentation and references: Detailed header comments? Yes

User guide or manual, technical reports, papers, books: "Subroutine Package for Processing Large Sparse Least-Squares Problems", William H Dillinger, NOAA Technical Memorandum, NOS, NGS-29, January 1981.

- 14. Approximate cost of obtaining software: \$45
- 15. Restrictions on use: None
- 16. Distributor: NOAA/NOS/NGS, National Geodetic Information Center, OA/C184 6001 Executive Blvd. Rockville, MD 20852 Phone (301) 443-8623

17. Original source of software:

Developer: W. H. Dillinger, R. H. Hanson

Institution: NOAA, NOS, National Geodetic Survey

U.S. Department of Commerce, NOAA, NOS, NGS

18. For further information contact: W. H. Dillinger

NOAA, NOS, National Geodetic Survey 6001 Executive Blvd. Rockville, MD 20852

Phone (301) 443-2520

1. Name of program or package: LSQR

Sparse linear system solver 2. Descriptive title:

Sparse linear least squares solver

Unsymmetric linear systems 3. Problem domain:

Overdetermined systems Damped least squares

4. Method of solution: Lanczos bidiagonalization

5. Programming language: ANSI FORTRAN

Single, easily converted to double 6. Precision:

Developed on IBM and Burroughs; 7. Portability:

easily portable to other machines

8. Other packages required:

9. Mode of use:

Callable subroutine

10. Test or demonstration program available? Yes

11. Length of code in lines: 574 Percentage comments: 66%

12. Special features: BLAS operations are efficient in a paging

environment and on pipeline machines. Overall efficiency may depend on user's own routine for computing y + Ax and $x + A^Ty$.

13. Documentation and references: **Detailed header comments?** Yes

User guide or manual, technical reports, papers, books:

Papers: C.C. Paige and M.A. Saunders, "LSQR: An algorithm for sparse

linear equations and sparse least squares", ACM TOMS 8, 1

(1982) 43-71.

C.C. Paige and M.A. Saunders, "Algorithm 583. LSQR: Sparse linear

equations and least squares problems", ACM TOMS 8, 2 (1982).

14. Approximate cost of obtaining software: See ACM Algorithms Order Form in ACM TOMS.

15. Restrictions on use: None

16. Distributor: ACM Algorithms Distribution Service

IMSL, Inc.

Sixth Floor, NBC Building, 7500 Bellaire Blvd.

Houston, TX 77036 17. Original source of software:

Chris Paige Michael Saunders Developer: Institution:

McGill University Stanford University
Natural Sciences and Engineering Research Council of Canada; Sponsor:

DSIR, New Zealand; DOE, NSF, ONR.

18. For further information contact:

Michael Saunders

Department of Operations Research

Stanford University

Ph: (415)497-1875 Stanford, CA 94305

- 1. Name of program or package: RNCLIN
- 2. Descriptive title: "Sparse Linear Systems and Least Squares Solver"
- **3. Problem domain:** Real Systems of Linear Equations or Least Squares Problems using $\mathbf{1}_2$ norm. No restriction on coefficient matrix.
- 4. Method of solution: Accelerated Iterative Column Projection Methods.
- 5. Programming language: Fortran IV
- 6. Precision: Either
- **7. Portability:** Developed using IBM 360/370 computer. Is portable or easily modified for other machines.
- 8. Other packages required: Program to generate matrix equation or Least Squares Prob.
- 9. Mode of use: Callable Subroutine.
- 10. Test or demonstration program available? Yes.
- 11. Length of code in lines: 343 lines Percentage comments: 67 %
- **12. Special features:** Uses column packed storage for matrices can be modified to use secondary storage or generate columns as necessary (Would involve additional programming by user).
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

User's Guide.

Technical reports and papers as soon as published.

- 14. Approximate cost of obtaining software: To be determined based on cost.
- 15. Restrictions on use: Propriety.
- 16. Distributor: Dr. Larry F. Bennett
 Department of Mathematics, South Dakota State University
 Brookings, South Dakota 57007 (Phone: 1-605-688-6218)
- 17. Original source of software:

Developer: Dr. Larry F. Bennett

Institution: South Dakota State University
Sponsor: South Dakota State University

18. For further information contact:

Dr. Larry F. Bennett

Department of Mathematics

South Dakota State University

Brookings, South Dakota 57007

Office Phone: 1-605-688-6218 Home Phone: 1-605-692-2161

- 1. Name of program or package: RNRWIN
- 2. Descriptive title: "Sparse Linear System and Least Squares Solver"
- **3. Problem domain:** Real Systems of Linear Equations or Least Squares Problems using $\mathbf{1}_2$ norm. No restriction on coefficient matrix.
- 4. Method of solution: Accelerated Iterative Row Projection Methods.
- 5. Programming language: Fortran IV
- 6. Precision: Either
- **7. Portability:** Developed using IBM 360/370. Is portable or easily modified for other machines.
- 8. Other packages required: Program to generate matrix equation or Least Squares Prob.
- 9. Mode of use: Callable Subroutine
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 325 lines Percentage comments: 71 %
- **12. Special features:** Uses row-packed storage for matrices can be modified to use secondary storage or generate rows as needed (Would involve additional programming by user).
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

User's Guide

rechnical reports and papers as soon as published.

- 14. Approximate cost of obtaining software: To be determined based on cost.
- 15. Restrictions on use: Propriety
- 16. Distributor: Dr. Larry F. Bennett

Department of Mathematics, South Dakota State University Brookings, South Dakota 57007 (Phone: 1-605-688-6218)

17. Original source of software:

Developer: Dr. Larry F. Bennett

Institution: South Dakoata State University
Sponsor: South Dakota State University

18. For further information contact:

Dr. Larry F. Bennett

Department of Mathematics

South Dakota State University

Brookings, South Dakota 57007

Office Phone: 1-605-688-6218 Home Phone: 1-605-692-2161

- 1. Name of program or package: EISPACK
- 2. Descriptive title: A Package of Matrix Eigensystem Routines
- 3. Problem domain: Standard eigensystem problem (real and complex), generalized eigensystem problem (real), singular value decomposition
- 4. Method of solution: QR, LR, QL, rational QR, bisection, QZ, inverse iteration
- 5. Programming language: FORTRAN

- 6. Precision: Double on IBM 360, single on others
- 7. Portability: Specific version for each of several machines
- 8. Other packages required: None
- 9. Mode of use: Library of callable subroutines
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 10,000 Percentage comments: 50%
- 12. Special features: None
- 13. Documentation and references: Machine-readable document for each subroutine Detailed header comments? Yes

 User guide or manual, technical reports, papers, books:
 - B. T. Smith et al., Matrix Eigensystem Routines EISPACK Guide, Springer-Verlag, Lecture Notes in Computer Science, Vol. 6 (2nd ed,), 1976
 - B. S. Garbow et al., Matrix Eigensystem Routines EISPACK Guide Extension Springer-Verlag, Lecture Notes in Computer Science, Vol. 51, 1977
- 14. Approximate cost of obtaining software: \$75
- 15. Restrictions on use: None
- 16. Distributor: NESC, Argonne National Laboratory (312) 972-7250 IMSL, Houston, Texas (713) 772-1927
- 17. Original source of software: Handbook of Linear Algebra, Wilkinson & Reinsch (eds.)

Developer: Applied Mathematics Division **Argonne National Laboratory**

Sponsor: NSF, DOE

18. For further information contact:

Burton S. Garbow
Mathematics and Computer Science Division
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, Illinois 60439
Phone: (312) 972-7184

1. Name of program or package: BES

2. Descriptive title: Basic Eigenanalysis System - Symmetric

3. Problem domain: Large, sparse, generalized, symmetric, real

4. Method of solution: Block Lanczos with shifting

5. Programming language: FORTRAN 77

6. Precision: Single or double

7. Portability: Good

8. Other packages required: VMSYST, EZ-GAL (data management)

9. Mode of use: Independent program system, interactive

10. Test or demonstration program available? Included

11. Length of code in lines: % 100,000 Percentage comments: 40%

12. Special features: Problem oriented language, interactive problem description followed by batch analysis, spectral range (section) specification of desired eigenpairs

13. Documentation and references:

Detailed header comments? Moderate

User guide or manual, technical reports, papers, books:

"Basic Eigenanalysis System" (in preparation)

- 14. Approximate cost of obtaining software: Not yet available
- 15. Restrictions on use:
- 16. Distributor:

17. Original source of software:

Developer: Paul S. Jensen

Institution: Lockheed Missiles and Space Co.
Sponsor: Lockheed Missiles and Space Co.

18. For further information contact:

Paul S. Jensen Lockheed Research Laboratory 5233/255 3251 Hanover St. Palo Alto, CA 94304

- 1. Name of program or package: BLMAIN
- 2. Descriptive title: Eigenvalue/Eigenvector Computations
- 3. Problem domain: Large Symmetric Matrices
- 4. Method of solution: Block Lanczos Recursion with Limited Reorthogonalization
- 5. Programming language: FORTRAN
- 6. Precision: Double
- 7. Portability: IBM/168/3033
- 8. Other packages required: Eispack
- 9. Mode of use: Stand-alone (can easily be modified to callable subroutines)
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: ~1000 Percentage comments: ~55%
- 12. Special features: None

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

Book: Lanczos Algorithms for Large Symmetric Eigenvalue Computations by Jane Cullum and Ralph Willoughby.

Volume? in Progress in Scientific Computing Series ed.

G. Golub, H. Kreiss, S. Arbarbanel, R. Glowinski,

Birkhäuser Boston Inc. 1983

- 14. Approximate cost of obtaining software: Please contact authors
- 15. Restrictions on use: None
- 16. Distributor: Please contact authors

17. Original source of software:

Developer: Jane Cullum and Ralph A. Willoughby **institution:** IBM T.J. Watson Research Laboratory, Yorktown Heights, N.Y. 10598 **Sponsor:**

18. For further information contact:

Jane Cullum
IBM T.J. Watson Research Center
Yorktown Heights, N. Y. 10598
914-945-2227 (if no answer message may be left with dept. secretary at
914-945-2331)

1. Name of program or package: LMAIN & LVMAIN

2. Descriptive title: Eigenvalue/Eigenvector Computations

3. Problem domain: Large Symmetric Matrices

4. Method of solution: Lanczos method with no reorthogonalization

5. Programming language: FORTRAN

6. Precision: Double

7. Portability: IBM/168/3033

8. Other packages required: None (Needs Random Number Generator)

9. Mode of use: Stand-alone (can easily be modified to callable subroutines)

10. Test or demonstration program available? Yes

11. Length of code in lines: ~2100 Percentage comments: ~55%

12. Special features: None

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

Book: Lanczos Algorithms for Large Symmetric Eigenvalue Computations by Jane Cullum and Ralph Willoughby.

Volume? in Progress in Scientific Computing Series ed.
G. Golub, H. Kreiss, S. Arbarbanel, R. Glowinski,
Birkhäuser Boston Inc. 1983.

- 14. Approximate cost of obtaining software: Please contact authors
- 15. Restrictions on use: None
- 16. Distributor: Please contact authors

17. Original source of software:

Developer: Jane Cullum and Ralph A. Willoughby

Institution: IBM T.J. Watson Research Laboratory, Yorktown Heights, N. Y. 10598

Sponsor:

18. For further information contact:

Jane Cullum
IBM T.J. Watson Research Center
Yorktown Heights, N. Y. 10598
914-945-2227 (if no answer message may be left with dept. secretary at
914-945-2331)

1. Name of program or package: EA12

2. Descriptive title: Find a group of eigenvalues and vectors.

3. Problem domain: Sparse symmetric matrices.

4. Method of solution: Simultaneous iteration.

5. Programming language: Fortran 66.

6. Precision: Both single and double precision versions are available.

7. Portability: Fortran 66.

8. Other packages required: Harwell subroutines EA13, FA01, FM01, FM02.

9. Mode of use: Subroutine calls.

10. Test of demonstration program available: Yes.

11. Length of code in lines: 427 Percentage comments: 37%

(934 with dependencies)

12. Special features: Reverse communication makes its use particularly flexible.

13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

The code is based on a adaptation by J.K.Reid of the work of H.Rutishauser (1970) Simultaneous iteration methods for symmetric matrices. Numer. Math., **16**, 205–223.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii), (iii) (see appendix on Harwell Subroutine Library).
- 16. Distributor: S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.
- 17. Original source of software:

Developer: I.S.Duff.

Institution: A.E.R.E. Harwell. Sponsor: A.E.R.E. Harwell.

18. For further information contact: I.S.Duff or J.K.Reid.

1. Name of program or package: EA14

2. Descriptive title: Eigenvalue spectrum.

3. Problem domain: Sparse symmetric matrices.

4. Method of solution: Lanczos algorithm.

5. Programming language: Fortran 66.

6. Precision: Double precision.

7. Portability: Fortran 66.

8. Other packages required: Harwell subroutine FA01.

9. Mode of use: Subroutine calls.

10. Test of demonstration program available: Yes.

11. Length of code in lines: 648 Percentage comments: 29%

(756 with dependencies)

12. Special features: Automatically chooses the number of Lanczos steps necessary to have confidence that the spectrum in a given interval has been found.

13. Documentation and references:

Detailed header comments? Yes, for auxiliary routines.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

B.N.Parlett and J.K.Reid (1981), Tracking the progress of Lanczos' algorithm for the very large symmetric eigenproblem. I.M.A. J. Num. Anal., 1, 135–155.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (i), (ii), (iii), (iv) (see appendix on Harwell Subroutine Library).
- 16. Distributor: S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.

17. Original source of software:

Developer: J.K.Reid.

Institution: A.E.R.E. Harwell. **Sponsor:** A.E.R.E. Harwell.

1. Name of program or package: LASO2

2. Descriptive title: Eigenvalue Solver

3. Problem domain: Sparse Symmetric Eigenvalue Problems

4. Method of solution: The Lanczos Algorithm with Selective Orthognalization

5. Programming language: ANSI FORTRAN 66

6. Precision: Either

7. Portability: Completely Portable

8. Other packages required: None

9. Mode of use: Callable Subroutines

10. Test or demonstration program available? $_{
m Yes}$

11. Length of code in lines: 3288 Percentage comments: 45%

each precision

12. Special features:

Requires user supplied subroutines for matrix vector multiplication and temporary storage of the Lanczos vectors

13. Documentation and references:

Detailed header comments? ye

User guide or manual, technical reports, papers, books:

Scott, D. S., "Block Lanczos Software for Symmetric Eigenvalue Problems," Computer Sciences Division, Union Carbide Corporation, Nuclear Div., November 1979, ORNL/CSD-48

LASO2.DOC, a text file available with the package

14. Approximate cost of obtaining software: Tape fee from NESC

15. Restrictions on use: None Free from Author over ARPA net

16. Distributor: National Energy Software Center, Argonne National Lab CS.SCOTT@UTEXAS-20 on the ARPA net

17. Original source of software:

Developer: D. S. Scott

Institution: Oak Ridge National Lab

Sponsor: DOF

18. For further information contact:

David S. Scott Computer Sciences Dept. PAI 3.28 University of Texas at Austin Austin, TX 78712 1. Name of program or package: STLM

Sparse eigenvalue problem solver 2. Descriptive title:

3. Problem domain: Large, sparse, generalized, symmetric, and real eigenvalue

problems

4. Method of solution: The Lanczos method applied on a sequence of shifted and

inverted problems

5. Programming language: ANSI FORTRAN. (will also run as a FORTRAN 77 package).

6. Precision: Either (type converter available).

7. Portability: CDC Cyber 730, PRIME 550-II. Easily portable (has passed the

PFORT Verifier).

8. Other packages required: Includes all necessary code, but linear system solver part may be replaced by the user's own if it makes use of special algorithms or

Callable subroutine. data structures.

10. Test or demonstration program available? Yes.

11. Length of code in lines: 6500 Percentage comments: 46

12. Special features: Requires a direct access file or virtual memory for large

problems.

13. Documentation and references:

Detailed header comments? No

User guide or manual, technical reports, papers, books: User guide and

The Spectral Transformation Lanczos Method for the Numerical Solution of Large Sparse Generalized Symmetric Eigenvalue Problems, Math. of Comp., vol 35, no. 152, 1251-1268.

14. Approximate cost of obtaining software:

15. Restrictions on use:

Will try to get it published in

ACM TOMS. 16. Distributor:

17. Original source of software:

Developer: Thomas Ericsson and Axel Ruhe

Institution: University of Umea, Inst of Information Processing

Sponsor: The Swedish Institute of Applied Mathematics (partly)

18. For further information contact:

Thomas Ericsson University of Umeå

Institute of Information Processing

S-901 87 Umeå

Sweden

1. Name of program or package: Subroutine TRACMN

2. Descriptive title: Generalized Eigenvalue Routine Using Trace

Minimization and Shifting

3. Problem domain: Generalized eigenvalues, real, symmetric, only matrix-vector multiply required

4. Method of solution: Trace minimization

5. Programming language: FLECS (FORTRAN)

6. Precision: Single

7. Portability: 66 Standard

8. Other packages required: BLAS, LINPACK, EISPACK, URAND (Forsythe

Malcom & Moler)

9. Mode of use: Subroutine call

10. Test or demonstration program available? Yes

11. Length of code in lines: 586 Percentage comments: 30%

12. Special features:

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

University of Illinois Report UIUCDCS-R-81-1056 Feb. 1981 SIAM J. Num. Analysis, Dec. 1982.

or

14. Approximate cost of obtaining software: None

15. Restrictions on use: None

16. Distributor: Authors

17. Original source of software:

Developer: John A. Wisniewski University of Illinois

Sponsor: NSF

18. For further information contact:

John A. Wisniewski Division 2113 Sandia National Laboratories Albuquerque, NM 87185 Ahmed H. Sameh Dept. of Computer Science University of Illinois 1304 W. Springfield Urbana, IL 61801 1. Name of program or package: SIMITZ

- **2. Descriptive title:** Eigenvectors and eigenvalues of real generalized symmetric matrices by simultaneous iteration.
- 3. Problem domain: Structural analysis, numerical weather prediction.
- 4. Method of solution: Subspace iteration (Rutishauser-Reinsch algorithm)
- **5. Programming language:** Version 1 FORTRAN 66 Version 2 FORTRAN 78
- 6. Precision: Single (Easily converted to double)
- 7. Portability: Control Data Corporation Cyber, fully portable.
- 8. Other packages required: Version 1 EISPACK, Version 2 SLATEC
- 9. Mode of use: Callable subroutine.
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 550 Percentage comments: 40%
- 12. Special features: Program is easily adaptable to vector or array processors.
- 13. Documentation and references:

 Detailed header comments? Yes

 User guide or manual, technical reports, papers, books:

Paul J. Nikolai, ALGORITHM 538 - Eigenvectors and eigenvalues of real generalized symmetric matrices by simultaneous iteration, ACM Trans. Math. Software 5 (1979), 118-125.

- **14.** Approximate cost of obtaining software: Version I Current IMSL fees.
- 15. Restrictions on use: None

Version II - None

16. Distributor: Version I - IMSL

7500 Bellaire Blvd Houston, TX 77036 (713) 772-1927 Version II - Paul J. Nikolai AFWAL/FIBR Wright-Patterson AFB OH 45433 (513) 255-5350

17. Original source of software:

Developer: Paul J. Nikolai

Institution: US Air Force Wright Aeronautical Laboratories

Sponsor: Air Force Systems Command

18. For further information contact:

Paul J. Nikolai AFWAL/FIBR Wright-Patterson AFB, OH 45433 (513) 255-5350 Autovon 785-5350 1. Name of program or package: LA05

2. Descriptive title: Solves linear sets of equations.

3. Problem domain: Linear programming bases.

4. Method of solution: Sparse Bartels-Golub algorithm.

5. Programming language: IBM Fortran.

6. Precision: Both single and double precision versions are available.

7. Portability: Fortran 66 version available.

8. Other packages required: Harwell subroutine MC20.

9. Mode of use: Subroutine calls.

10. Test of demonstration program available: Yes.

11. Length of code in lines: 959 Percentage comments: 22%

(1062 with dependencies)

12. Special features: Markowitz' pivoting used for original factorization. If updating can be performed by permutations alone, without fill-in, then this is done.

13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

J.K.Reid (1976), Fortran subroutines for handling sparse linear programming bases, Harwell report R.8269, H.M.S.O., London.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii), (iii) (see appendix on Harwell Subroutine Library).
- **16. Distributor:** S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwel', Oxfordshire OX11 ORA, England.

17. Original source of software:

Developer: J.K.Reid.

Institution: A.E.R.E. Harwell. Sponsor: A.E.R.E. Harwell.

- 1. Name of program or package: SPLP
- 2. Descriptive title: Sparse linear programming subprogram
- 3. Problem domain: Linear optimization problems with general bounds on the variables (including no bounds) and linear constraints.
- 4. Method of solution: Basicly the Revised Simplex method.
- 5. Programming language: SFTRAN and FORTRAN 77
- 6. Precision: Single

- 7. Portability: Developed and used on CDC, usea on VAX and IBM.
- 8. Other packages required: BLAS, XERROR (SLATEC library error package)
- (copies in package)

 9. Mode of use: Callable subroutine
- 10. Test or demonstration program available? y_{es}
- 11. Length of code in lines: code 5600 (FORTR Reprentage comments: 10% comments document 1500
- 12. Special features: Permits out-of-core storage of data matrix (may require machine dependent I/O subprograms -- 3 types now provided) efficient design for paging, written in several subprograms so easily segmented.
- 13. Documentation and references: Yes.

Detailed header comments? Brief document and full.

User guide or manual, technical reports, papers, books:

"A Sparse Linear Programming Subprogram," R. J. Hanson, K. L. Hiebert, Sandia Technical Report SAND81-0297, Sandia National Labs, Albuquerque, NM 87185.

- 14. Approximate cost of obtaining software: Send tape with letter of request.
- 15. Restrictions on use: Rights to redistribute (modified) LAO5 within the package
- have been purchased.

 16. Distributor: Ultimately NESC
- 17. Original source of software:

Developer: R. J. Hanson, K. L. Hiebert

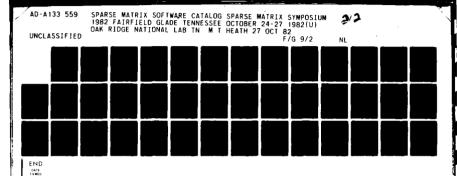
Institution: Sandia National Labs

Sponsor: DOE

18. For further information contact:

Dick Hanson.
Org. 5642
Sandia National Labs.
Albuquerque, NM 87185
(505) 844-1715
FTS 844-1715

Kathie Hiebert Org. 5642 Sandia National Labs. Albuquerque, NM 87185 (505) 844-3538 FTS 844-3538



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1. Name of program or package: XMP

2. Descriptive title: Hierarchically structured linear programming library

3. Problem domain: Linear Programming

4. Method of solution: Simplex Method

5. Programming tanguage: FORTRAN

6. Precision: Double (or single for Control Data)

7. Portability: Any FORTRAN compiler-highly portable

8. Other packages required: LAØ5 package from Harwell

9. Mode of use: Subroutine Library

10. Test or demonstration program available? Yes

11. Length of code in lines: 20,000 Percentage comments: 50%

12. Special features: primal and dual simplex methods;

simple and generalized upper bounds;

postoptimality analysis

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

"The Design of the XMP Library", Transactions on Mathematical Software, Vol. 7, No. 4, December, 1981.

- 14. Approximate cost of obtaining software: negotiable
- 15. Restrictions on use: negotiable
- 16. Distributor: Management Information Systems Dept.

University of Arizona

17. Original source of software:

Developer: Roy Marsten

Institution: NBER/MIT/University of Arizona

Sponsor: NSF

18. For further information contact:

Professor Roy Marsten Management Information Systems Dept. University of Arizona Tucson, Arizona - 85721

- 1. Name of program or package: SIMPLE
- 2. Descriptive title: Sparse linear programming problem solver
- 3. Problem domain: Linear programming
- 4. Method of solution Pevised simplex
- 5. Programming language: AP FORTRAN and FPS-164 assembly language
- 6. Precision: 64-bit word
- 7. Portability: Developed for the FPS-164 Array Processor.
- 8. Other packages required: FPS-164 Math Library (APMATH64)
- 9. Mode of use: Callable subroutine
- 10. Test or demonstration program available? No
- 11. Length of code in lines: 558

- Percentage comments: 63
- 12. Special features: Takes advantage of the parallel, pipelined architecture of the FPS-164 array processor.
- 13. Documentation and references: Detailed header comments? Yes

User guide or manual, technical reports, papers, books: APMATH64 Reference Manual Floating Point Systems, Inc.

- 14. Approximate cost of obtaining software: This routine is included in the FPS-164
- Math Library (APMATH64)

 15. Restrictions on use: License agreement required
- 16. Distributor: Floating Point Systems, Inc.

P.O. Box 23489 Portland, OR 97223

17. Original source of software:

Developer: Ron Coleman

Institution: Floating Point Systems, Inc. Sponsor: Floating Point Systems, Inc.

18. For further information contact:

Phil Vaughn Floating Point Systems, Inc. P.O. Box 23489 Portland, OR 97223 (503) 641-3151 TLX: 360470 FLOATPOIN BEAV

- 1. Name of program or package: P3, P4
- 2. Descriptive title: Subroutines for Hellerman-Rarick P³ and P⁴ algorithms
- 3. Problem domain: Useful in codes for linear programming and solving sparse nonlinear equations via tearing.
- 4. Method of solution: "Symbolic" computation on arrays of integers.
- 5. Programming language: IBM Fortran with simple conversion to ANSI Fortran.
- 6. Precision: Single or double -- no floating-point data are used.
- 7. Portability: Developed on IBM 370/168; acceptable to PFORT Verifier (after simple conversion)
- 8. Other packages required: Harwell Library subroutines MC13D, MC21A
- 9. Mode of use: Subroutine call; P4 calls P3.
- 10. Test or demonstration program available? N_0 .
- 11. Length of code in lines: 684 Percentage comments: 45.8%
- 12. Special features: Some integer arrays can be "short" integers -- INTEGER*2 in IBM Fortran. Changing "INTEGER*2" to "INTEGER" is the simple conversion mentioned above.
- 13. Documentation and references:

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Detailed header comments? Yes.

User guide or manual, technical reports, papers, books: references:

- E. Hellerman and D.C. Rarick, "The Partitioned Preassigned Pivot Procedure (P⁴)", pp. 67-76 of <u>Sparse Matrices and Their Applications</u>, edited by D.J. Rose and R.A. Willoughby, Plenum Press, New York, 1972.
- E. Hellerman and D.C. Rarick, "Reinversion with the Preassigned Pivot Procedure", Math. Programming 1 (1971), pp. 195-216.
- 14. Approximate cost of obtaining software: no fee
- 15. Restrictions on use: none
- 16. Distributor: see item 18.
- 17. Original source of software:

Developer: David M. Gay

Institution: Center for Computational Research in Economics and Management Science,

Sponsor: NSF Massachusetts Institute of Technology.

18. For further information contact: David M. Gay

Bell Labs

600 Mountain Avenue Murray Hill, NJ 07974

phone: (201) 582-5623

1. Name of program or package: MINOS - HP

2. Descriptive title: Linear Programming Package for HP1000

3. Problem domain: Linear Programming

4. Method of solution: Simplex method

5. Programming language: FORTRAN

6. Precision: Single

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7. Portability: HP1000F; portable (see 12 below)

8. Other packages required:

9. Mode of use: Stand-alone

10. Test or demonstration program available? Yes

11. Length of code in lines: 6700 Percentage comments: 5%

12. Special features: Stores large array, Z(25000), in (paged) memory;

some machine-dependent routines

13. Documentation and references:

Detailed header comments? No

User guide or manual, technical reports, papers, books: MINOS User Guide MINOS System Manual

14. Approximate cost of obtaining software: TBA

15. Restrictions on use: TBA

16. Distributor: TBA

17. Original source of software:

Developer: Michael Saunders, Systems Optimization Laboratory

Institution: Stanford University

Sponsor: U.S. and New Zealand governments

18. For further information contact: James E. Giles

Tennessee Valley Authority

P.O. Drawer E

Norris, Tennessee 37828

(FTS) 856-4460

1. Name of program or package: NS03

2. Descriptive title: Solves non-linear sets of equations.

3. Problem domain: Equations with sparse Jacobian matrices.

4. Method of solution: Marquardt's algorithm.

5. Programming language: IBM Fortran.

6. Precision: Both single and double precision versions are available.

7. Portability: Fortran 66 version available.

8. Other packages required: Harwell subroutines MA17, FM01, MC09, TD02.

9. Mode of use: Subroutine calls.

10. Test of demonstration program available: Yes.

11. Length of code in lines: 668 Percentage comments: 24%

(1034 with dependencies)

12. Special features: Provision of derivatives is optional.

13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

J.K.Reid (1972) Fortran subroutines for the solution of sparse systems of non-linear equations. Harwell report R-7293, H.M.S.O., London.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii) and (iii) (see appendix on Harwell Subroutine Library).
- **16. Distributor:** S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.

17. Original source of software:

Developer: J.K.Reid.

Institution: A.E.R.E. Harwell. **Sponsor:** A.E.R.E. Harwell.

1. Name of program or package: VA08

2. Descriptive title: Function minimization.

3. Problem domain: Functions with sparse Hessian matrices.

4. Method of solution: Conjugate gradients.

5. Programming language: Fortran 66.

6. Precision: Both single and double precision versions are available.

7. Portability: Fortran 66

8. Other packages required: Harwell subroutine FM02.

9. Mode of use: Subroutine calls.

10. Test of demonstration program available: Yes.

11. Length of code in lines: 86 Percentage comments: 1%

(211 with dependencies)

12. Special features:

13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

R.Fletcher and C.M.Reeves (1964) Function minimization by conjugate gradients. Comp. J. 7, 149–154.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii), (iii) (see appendix on Harwell Subroutine Library).
- **16. Distributor:** S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.

17. Original source of software:

Developer: R.Fletcher.

Institution: Univ. of Dundee. **Sponsor:** A.E.R.E. Harwell.

1. Name of program or package: VA14

2. Descriptive title: Function minimization.

3. Problem domain: Functions with sparse Hessian matrices.

4. Method of solution: Conjugate gradients.

5. Programming language: Fortran 66.

6. Precision: Both single and double precision versions are available.

7. Portability: Fortran 66.

8. Other packages required: None.

9. Mode of use: Subroutine calls.

10. Test of demonstration program available: Yes.

11. Length of code in lines: 191 Percentage comments: 13%

12. Special features: Automatic restart procedure included.

13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

M.J.D.Powell (1977) Restart procedures for the conjugate gradient method. Math. Prog. 12, 241–254.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii), (iii) (see appendix on Harwell Subroutine Library).
- **16. Distributor:** S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.

17. Original source of software:

Developer: M.J.D.Powell.

Institution: Univ. of Cambridge. Sponsor: A.E.R.E. Harwell.

1. Name of program or package: VE05

2. Descriptive title: Minimization subject to linear constraints.

3. Problem domain: Sparse constaint matrix.

4. Method of solution: Variable metric algorithm.

5. Programming language: IBM Fortran.

6. Precision: Both single and double precision versions are available.

7. Portability: Fortran 66 version available.

8. Other packages required: Other Harwell subroutines.

9. Mode of use: Subroutine calls.

10. Test of demonstration program available: Yes.

11. Length of code in lines: 1075 Percentage comments: 16%

(3022 with dependencies)

12. Special features: Essentially extends sparse linear programming techniques to non-linear objective functions.

13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

A.Buckley (1975) An alternate implementation of Goldfarb's minimization algorithm. Math. Prog. 8, 207–231.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii), (iii) (see appendix on Harwell Subroutine Library).
- 16. Distributor: S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.

17. Original source of software:

Developer: A.Buckley.

Institution: Concordia Univ., Montreal.

Sponsor: A.E.R.E. Harwell.

1. Name of program or package: MINOS

2. Descriptive title: Sparse nonlinear programming system

Optimization involving a nonlinear objective function,

bounds, and linear and nonlinear constraints.

4. Method of solution: Simplex method for linear programs; reduced-gradient

method + quasi-Newton for linear constraints;

5. Programming language: projected Lagrangian method for nonlinear constraints.

FORTRAN IV

6. Precision: Single or mixed, depending on machine.

7. Portability: Developed on IBM; easily portable to other (large)

machines.

8. Other packages required:

None

9. Mode of use: Stand-alone, primarily; callable by expert user.

10. Test or demonstration program available? Yes

11. Length of code in lines: 10,000 Percentage comments: 35%

12. Special features: In-core solution procedure; designed for efficiency

in a paging environment; disk files used to input

data and save current solution.

13. Documentation and references:

Detailed header comments? No

User guide or manual, technical reports, papers, books:

User manuals: reports SOL 77-9, 77-31, 80-14, 80-15, 80-100,

Department of Operations Research, Stanford University.

Papers: Mathematical Programming 14 (1978) 41-72.

Mathematical Programming Study 16 (1982) 84-117.

14. Approximate cost of obtaining software: \$300 academic; \$3000 commercial.

15. Restrictions on use: License agreement required.

16. Distributor: Office of Technology Licensing

105 Encina Hall Stanford University

Stanford Cali

Stanford, California 94305 Ph: (415)497-0651

17. Original source of software:

Developer:Institution:

Bruce A. Murtagh Michael A. Saunders
University of NSW Stanford University

Sponsor: DOE, NSF, ONR, ARO

18. For further information contact:

Technical details: Michael Saunders, Dept. of Operations Research,

Stanford University, Stanford, CA 94305. (415)497-1875

Distribution: Bill Osborn, Office of Technology Licensing

(see 16 above)

- 1. Name of program or package: TD02
- 2. Descriptive title: Evaluates an approximate Jacobian matrix.
- 3. Problem domain: Must be given a function f(x).
- 4. Method of solution: First central differences with an automatic choice of step-size.
- 5. Programming language: IBM Fortran.
- 6. Precision: Both single and double precision versions are available.
- 7. Portability: Fortran 66 version available.
- 8. Other packages required: None.
- 9. Mode of use: Subroutine calls.
- 10. Test of demonstration program available: Yes.
- 11. Length of code in lines: 237 Percentage comments: 18%
- 12. Special features: May or may not be given the sparsity pattern. Uses the sparsity to economize on function calls.
- 13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

A.R.Curtis, M.J.D.Powell and J.K.Reid (1974) On the estimation of sparse Jacobian matrices. J. Inst. Math. Applics. **13,** 117–120.

A.R.Curtis and J.K.Reid (1974) The choice of step lengths when using differences to approximate Jacobian matrices. J. Inst. Math. Applics 13, 121-126.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii), (iii) (see appendix on Harwell Subroutine Library).
- 16. Distributor: S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.
- 17. Original source of software:

Developer: J.K.Reid.

Institution: A.E.R.E. Harwell. **Sponsor:** A.E.R.E. Harwell.

18. For further information contact: The developer.

1. Name of program or package: TD03

2. Descriptive title: Evaluates an approximate Hessian matrix.

3. Problem domain: Sparse Hessian matrices.

4. Method of solution: Finite differences.

5. Programming language: Fortran 66.

6. Precision: Double precision.

7. Portability: Fortran 66.

8. Other packages required: None.

9. Mode of use: Subroutine calls.

10. Test of demonstration program available: Yes.

11. Length of code in lines: 882 Percentage comments: 53%

12. Special features: Uses sparsity to economize function calls.

13. Documentation and references:

r ailed header comments? Yes, for auxiliary routines.

User guide or manual, technical reports, papers, books:

Harwell Subroutine Library Specification Document.

M.J.D.Powell and P.L.Toint (1979) On the estimation of sparse Hessian matrices. S.I.A.M. J.

Numer. Anal. 16, 1060-1074.

- 14. Approximate cost of obtaining software: See appendix on Harwell Subroutine Library.
- 15. Restrictions on use: (ii), (iii) (see appendix on Harwell Subroutine Library).
- 16. Distributor: S. Marlow, CSS Division, Building 8.9, A.E.R.E. Harwell, Oxfordshire OX11 ORA, England.

17. Original source of software:

Developer: P.L.Toint and I.S.Duff.

Institution: Univ. of Namur and A.E.R.E. Harwell.

Sponsor: Univ. of Namur and A.E.R.E. Harwell.

18. For further information contact: I.S.Duff.

- 1. Name of program or package: DSM
- 2. Descriptive title: Package for estimating a sparse Jacobian matrix with a minimal or nearly minimal number of function evaluations.
- 3. Problem domain: DSM partitions the columns of a sparse matrix into groups so that columns in a given group do not have a nonzero in the same row position.
- 4. Method of solution: The partitioning problem is associated with an equivalent graph coloring problem, and graph coloring heuristics are used to solve the partitioning problem.
- 5. Programming language: ANSI Fortran 66
- 6. Precision: Not applicable. Only integer arithmetic used.
- 7. Portability: Machine independent.
- 8. Other packages required: None
- 9. Mode of use: Callable subroutine
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 1470 Percentage comments: 67%
- 12. Special features: DSM is designed to produce optimal or nearly optimal results. DSM is called once to analyze the sparsity structure of the Jacobian matrix. DSM then produces the partitioning information needed to estimate the Jacobian matrix. This information is stored in an integer array of length equal to the number of variables.
- 13. Documentation and references:

Detailed header comments? Ye

User guide or manual, technical reports, papers, books:

Coleman, T. F. and Moré, J. J. [1981]. Estimation of sparse Jacobian matrices and graph coloring problems, Argonne National Laboratory, Report ANL-81-39. To appear in SIAM J. Numerical Analysis.

Coleman, T. F. and Moré, J. J. [1982]. Software for estimating sparse Jacobian matrices, Argonne National Laboratory, Report ANL-82-37.

- 14. Approximate cost of obtaining software: Determined by NESC
- 15. Restrictions on use: None
- 16. Distributor: National Energy Software Center (NESC)
- 17. Original source of software:

Developer: Coleman, T. F., Garbow, B. S., and Moré, J. J.

Institution: Argonne National Laboratory

Sponsor: DOE

18. For further information contact:

B. S. Garbow
Mathematics and Computer Science Division
Argonne National Laboratory
Argonne, Illinois 60439
(312) 972-7184 (FTS):972-7184

1. Name of program or package: MFLPP

2. Descriptive title: Continuous Minisum Multifacility Location Problem

Solver

3. Problem domain: Unconstrained $\ell_{\mathbf{p}}$ distance problems

4. Method of solution: Projected Newton Method

5. Programming language: ANSII FORTRAN

6. Precision: Single

7. Portability: Runs through PFORT verifiew

8. Other packages required: None

9. Mode of use: Callable subroutines

10. Test or demonstration program available? Not yet

11. Length of code in lines: Percentage comments:

12. Special features: Ability to handle certain constraints to be added

in the near future

13. Documentation and references:

Detailed header comments? No

User guide or manual, technical reports, papers, books:

Paper: "A Second-order method for sol ving the continuous multifacility location problem," Paul Calamai and Andrew Conn, Proceedings of the 1981 Dundee Conference in Numerical Analysis (to appear).

14. Approximate cost of obtaining software: Mail + tape (research); To be determined (commercial).

15. Restrictions on use: None (research);

16. Distributor: To be determined (commercial)

(See 18.)

17. Original source of software:

Developer: Paul Calamai and Andrew Conn

Institution: University of Waterloo, Waterloo, Ontario, CANADA

Sponsor: NSERCC

18. For further information contact:

A. R. Conn. Department of Computer Science

P. H. Calamai, Department of Systems Design

University of Waterloo

Waterloo, Ontario, CANADA N21 3G1

- 1. Name of program or package: EPO 1
- 2. Descriptive title: Entropy problem solver.
- 3. Problem domain: Maximization of entropy subject to sparse linear equality and inequality constraints. Applications in regional science, traffic planning, etc.
- 4. Method of solution: The Newton conjugate gradient method.
- 5. Programming language: ANSI FORTRAN
- 6. Precision: Single and double.
- 7. Portability: Developed on DEC 10. Easily portable.
- 8. Other packages required: None.
- 9. Mode of use: Callable subroutine.
- 10. Test or demonstration program available? Y_{es} .
- 11. Length of code in lines: 1200 Percentage comments: 65%
- 12. Special features: -

13. Documentation and references:

Detailed header comments? Yes.

User guide or manual, technical reports, papers, books:

Jan Eriksson, Algorithms for entropy and mathematical programming, Linköping Studies in Science and Technology Dissertations No.63 Linköping University, Sweden.

- 14. Approximate cost of obtaining software: Free for none commercial use.
- 15. Restrictions on use: License agreement required for commercial use.
- 16. Distributor:
- 17. Original source of software:

Developer: Jan Eriksson

Institution: Department of Mathematics, Linköping University

Sponsor:

18. For further information contact: Jan Eriksson

Department of Mathematics

Linköping University, S-581 83 Linköping

Sweden. Phone: 46-111700

- 1. Name of program or package:
- 2. Descriptive title: Input-Output Model of the World Economy
- 3. Problem domain: Nonsymmetric sparse bordered block diagonal linear systems in each time period
- 4. Method of solution: Block Gauss in each system, direct method for each block
- 5. Programming language: ANSI FORTRAN
- 6. Precision: Available in single and double precision
- 7. Portability: Developed on IBM, but only used standard FORTRAN to make it very portable-IBM version with half length integer also available
- 8. Other packages required: LINPACK, MA28 set from Harwell
- 9. Mode of use: Driver program and 36 subroutines (18 of which are from the
- 10. Test or demonstration program available?

above mentioned packages)

- 11. Length of code in lines: 5000 including Percentage comments: 40% 2000 from packages
- 12. Special features: special "global" storage scheme

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books: (1) World Model Program Documentation-Release 1, July 1982; (2) Daniel B. Szyld-Using Sparse Matrix Techniques to solve a model of the World Economy, in I.S. Duff (ed.) Sparse Matrices and their Uses, Academic Press, London, 1981, pp. 357-365; (3) Faye Duchin and Daniel B. Szyld, Application of Sparse Matrix Techniques to Inter Regional Input-Output Analysis-Economics of Planning, 15 (1979) pp.142-167.

- 14. Approximate cost of obtaining software: To discuss in each case
- 15. Restrictions on use: Agreement required
- 16. Distributor: Same as 18.

17. Original source of software:

Developer: Daniel B. Szyld

Institute for Economic Analysis, New York University

Sponsor:

18. For further information contact:

Daniel B. Szyld Institute for Economic Analysis New York University 269 Mercer Street New York, N.Y. 10003 Phone: (212) 598-3413

- 1. Name of program or package: CONOPT
- 2. Descriptive title: Large Scale Optimal Control System
- 3. Problem domain: Time-dependent optimization problems with linear/nonlinear objective, linear/nonlinear constraints, and bounds.
- 4. Method of solution: Reduced gradient relying on sparsity and staircase structure.
- 5. Programming language: FORTRAN
- 6. Precision: Single and double
- 7. Portability: Developed on CDC. Other versions are being developed.
- 8. Other packages required: none
- 9. Mode of use: Stand-alone job control procedure
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 20,000 Percentage comments: 40
- 12. Special features:

13. Documentation and references:

Detailed header comments?

User guide or manual, technical reports, papers, books:

CONOPT - A System for Large Scale Dynamic Nonlinear Optimization, User's Guide, Arne Drud and Alex Meeraus, Development Research Center, World Bank, 1818 H Street, N.W., Washington, D.C., 20433, U.S.A.

- 14. Approximate cost of obtaining software: negotiable
- 15. Restrictions on use: license agreement required
- 16. Distributor: See 18
- 17. Original source of software:

Developer: Arne Drud

Institution: Development Research Department, World Bank

Sponsor:

18. For further information contact:

Arne Drud
Development Research Department
The World Bank
1818 H Street, N.W.
Washington, D.C. 20433
U.S.A.
Phone - (202) 676-1034

1. Name of program or package: NLPNET

2. Descriptive title: Large- Scale LINEAR and Nonlinear Network Flow Optimization

3. Problem domain: Minimization of separable functions subject to network flow constraints (water distribution, electrical power network

4. Method of solution:

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optimization, Econometrics)

5. Programming language: Fortran IV

6. Precision: Single or Double 7. Portability: CDC, IBM, DEC

8. Other packages required: NONE

9. Mode of use: Callable subroutine, stand alone main also included

10. Test or demonstration program available?

11. Length of code in lines: 6,000

Percentage comments: 40%

12. Special features: Can take advantage of machines supporting INTEGER * 2 to reduce storage significantly.

13. Documentation and references:

Detailed header comments?

User guide or manual, technical reports, papers, books:

User guide, technical reports

14. Approximate cost of obtaining software: \$300.00 for research

None (research). Varies for commercial use. 15. Restrictions on use:

16. Distributor:

License agreement (commercial).

SOM, Yale University, Box 1A, New Haven, CT 06520 Ph. (203) 436-1952

17. Original source of software:

Developer: R. Dembo

Institution: Yale University **Sponsor:** (In part) NSF

Ron Dembo

18. For further information contact:

Ron Dembo

SOM

Yale University

Box 1A

New Haven, CT 06520

- 1. Name of program or package: FACSIMILE
- 2. Descriptive title: Simulator for mass action kinetics with diffusion/advection, and other initial value problems.
- 3. Problem domain: Stiff ODE, including large problems.
- **4. Method of solution:** Backward Difference Formula, with sparse matrix handling by Harwell MA28 package (non-symmetric, minimum degree).
- **5. Programming language:** Written in Fortran 66. Provides user with Problem-Oriented High Level Language.
- **6. Precision:** User-specified. Default 10^{-3} .
- 7. Portability: Available on IBM, Amdahl, Perkins-Elmer; Cray; ICL 29XX; DEC VAX. Others considered.
- 8. Other packages required: All included.
- 9. Mode of use: Background or foreground.
- 10. Test or demonstration program available? Package of \sim 10 test problems.
- 11. Length of code in lines: ~ 21,000. Perce

Percentage comments: Small.

- **12. Special features:** Complete package providing command language and high-level programming language, with powerful input/output features, all in a single job step. Optimisation (parameter-fitting) features.
- 13. Documentation and references:
 Detailed header comments? No.
 User guide or manual, technical reports, papers, books:

User manual (with updates). Implementation Manual. Reports on applications in certain cases.

- 14. Approximate cost of obtaining software: \$5,000 for indefinite license.
- 15. Restrictions on use: Single CPU. Special terms for more than one.
- 16. Distributor: A.E.R.E. Harwell,
 Didcot,
 Oxon OX11 ORA, England.
- 17. Original source of software: A.E.R.E. Harwell.

 Developer: Applied Mathematics Group, A.E.R.E.
 Institution: A.E.R.E.
 Sponsor: U.K.A.E.A.
- 18. For further information contact: (a) A.R. Curtis,
 Computer Science and Systems Division,
 A.E.R.E.
 - (b) Commercial Officer, C.S.S.D. A.E.R.E.

1. Name of program or package: GEARBI

2. Descriptive title: Solves initial value problem for ODE system having a blocked sparse Jacobian

- 3. Problem domain: Stiff or nonstiff systems, given in explicit form y = f(t,y) with regular block structure
- 4. Method of solution: Adams or BDF integration, with block-SOR for linear system solution
- 5. Programming language: FORTRAN IV
- 6. Precision: Single
- 7. Portability: Developed on CDC-7600, but reasonably portable
- 8. Other packages required: None
- 9. Mode of use: Callable subroutine
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: appx, 1350 Percentage comments: 43%
- 12. Special features: Internal Common blocks require redimensioning for large problems. Relaxing assumptions about block structure requires changes in one routine.
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

A. C. Hindmarsh, "Preliminary Documentation of GEARBI: Solution of ODE Systems with Block-Iterative Treatment of the Jacobian," LLNL Report UCID-30149, December 1976.

- 14. Approximate cost of obtaining software: None
- 15. Restrictions on use: None
- 16. Distributor: Same as 18.
- 17. Original source of software:

Developer: Alan C. Hindmarsh

Institution: LLNL Sponsor: DOE

18. For further information contact:

Alan C. Hindmarsh
Mathematics and Statistics Division, L-316
Lawrence Livermore National Laboratory
Livermore, California 94550
Phone: (415) 422-4276

(415) 422-4276 FTS - 532-4276

- 1. Name of program or package: LSODES
- 2. Descriptive title: Solves initial value problem for ODE system having a general sparse Jacobian
- 3. Problem domain: Stiff or nonstiff systems, given in explicit form $\dot{y} = f(t,y)$
- **4. Method of solution:** Adams or BDF integration, with YSMP (Yale Sparse Matrix Package) for linear system solution
- 5. Programming language: FORTRAN IV
- 6. Precision: Both single and double precision versions (separate) available
- 7. Portability: Developed on CDC-7600 but designed to be highly portable
- 8. Other packages required: [YSMP (ODRV and CDRV) supplied with package]
- 9. Mode of use: Callable subroutine
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: apprx. 5400 Percentage comments: 55%
- 12. Special features: Easy to use in dump/restart or overlay mode

13. Documentation and references:

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Detailed header comments? Yes (this is the only usage manual at present)
User guide or manual, technical reports, papers, books:

A. C. Hindmarsh, "Toward a Systematized Collection of ODE Solvers," in the Proceedings of the 10th IMACS World Congress, 1982 (in process).

- 14. Approximate cost of obtaining software: None
- 15. Restrictions on use: None
- 16. Distributor: Same as 18.
- 17. Original source of software: (excluding development of YSMP)

Developer: Alan C. Hindmarsh(LLNL), Andrew H. Sherman (Exxon Prod. Res. Co.)

Institution: LLNL Sponsor: DOE

18. For further information contact:

Alan C. Hindmarsh
Mathematics and Statistics Division, L-316
Lawrence Livermore National Laboratory
Livermore, California 94550
Phone: (415) 422-4276
FTS - 532-4276

1. Name of program or package: LSOD28

Stiff ODE Solver for Sparse Systems 2. Descriptive title:

- 3. Problem domain: Stiff ODE initial value problems with particular application to problems having a general large sparse Jacobian matrix.
- 4. Method of solution: Gear's backward differentiation formulas. LU decomposition.
- 5. Programming language: FORTRAN
- **6. Precision:** Single and double precision; standard FORTRAN, IBM FORTRAN using INTEGER*2 representation.
- 7. Portability: Developed on IBM; designed to be easily portable
- 8. Other packages required: Proprietary package MA28
- 9. Mode of use: Callable subroutine
- 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 3000 Percentage comments:
- 12. Special features: Option of using INTEGER*2 representation for integer arrays on IBM machines.
- 13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

LSOD28: A Variant of LSODE for Problems Having a General Large Sparse Jacobian Matrix by Richard L. Cox, K/CSD-16 (October 1982).

- 14. Approximate cost of obtaining software: LSOD28, nominal; MA28, \$400
- 15. Restrictions on use: None on LSOD28; MA28 proprietary.
- 16. Distributor: National Energy Software Center

LSOD28:

Argonne National Laboratory 9700 South Cass Avenue Argonne, Illinois 60439

MA28:

Harwell Subroutine Library

Building 8.9 AERE Harwell Oxon OXII ORA England

17. Original source of software:

Developer: Richard L. Cox

Institution: Oak Ridge Gaseous Diffusion Plant, Oak Ridge, TN

Sponsor: DOE

18 For further information contact:

Richard L. Cox Union Carbide Corporation Nuclear Division P. O. Box P, Bldg. K-1007 Oak Ridge, TN 37830

Phone: Commercial 615/574-8726 FTS 624-8726

1. Name of program or package: SPARKS

2. Descriptive title: Stiff ODE package

3. Problem domain: Large systems of ODE's with Sparse Jacobians

4. Method of solution: Semi Implicit Runge Kutta method

5. Programming language: FORTRAN

6. Precision: Single IBM-3033

7. Portability: Developed for IBM-3033 but has been transformed to UNIVAC

8. Other packages required: Uses SSLEST for Sparse Matrix Factorization

9. Mode of use: Callable subroutine package includes 5 subroutines

10. Test or demonstration program available?

11. Length of code in lines: 1100 lines of Percentage comments: 25% comments code

12. Special features: Uses efficient Jacobian evaluation.

Applies drop tolerance and iterative refinement.

Variable stepsize control

13. Documentation and references:

Detailed header comments?

User guide or manual, technical reports, papers, books:

Users guide: N. Houbak & P.G. Thomsen SPARKS - A Fortran subroutine for the solution of Large Systems of Stiff ODE;s with Sparse Jacobians. NI-79-02

14. Approximate cost of obtaining software: \$ 50

15. Restrictions on use: Non commercial

19. Nestrictions on pae. Horr commercial

16. Distributor: Dept. for Numerical Analysis

Bulding 303

Technical University of Denmark, DK-2800 Lyngby, Denmark

17. Original source of software:

Developer: Institution:

N. Houbak - P.G. Thomsen

Dept. for Numerical Analysis, Technical Univ. of Denmark

Sponsor:

18. For further information contact:

Per Grove Thomsen

Dept. for Numerical Analysis, Bulding 303

Technical University of Denmark, DK-2800 Lyngby

DENMARK, Tel. 881911 ext. 4373

- 1. Name of program or package: LARKIN
- 2. Descriptive title: simulation package for large chemical reaction systems
- 3. Problem domain: solution of very large systems of stiff ODE's arising from chemical kinetics
- 4. Method of solution: stiff extrapolation integrator using adapted sparse matrix techniques
- 5. Programming language: standard FORTRAN (ANSI-FORTRAN with few extensions)
- 6. Precision: either

- 7. Portability: developed on IBM 370/168, easily portable to other machines
- 8. Other packages required: none
- 9. Mode of use: main program with subroutines
- 10. Test or demonstration program available?
- 11. Length of code in lines: 8300

Percentage comments: 35%

12. Special features: segmented for OVERLAY

package designed especially for interactive use

13. Documentation and references:

Detailed header comments?

User guide or manual, technical reports, papers, books:

Deuflhard, Bader, Nowak: LARKIN - a software package for the numerical simulation of LARge systems ...; Univ. Heidelberg T.Report 100 (1980) Bader, Nowak, Deuflhard: An advanced simulation package for large chemical reaction systems; Univ. Heidelberg, T.Rep. 149 (1982) Duff, Nowak: On sparse matrix techniques in ...; T.Rep. (1982)

- 14. Approximate cost of obtaining software: not yet decided
- 15. Restrictions on use: licence agreement required
- 16. Distributor: Prof. Dr. P. Deuflhard

Universität Heidelberg, Institut f. Angewandte Mathematik D-6900 Heidelberg, W. Germany

17. Original source of software:

Developer:

U. Nowak, G. Bader, P. Deuflhard

Institution: Inst. f. Applied Mathematics, Universität Heidelberg

Sponsor: DFG (SFB 123)

18. For further information contact:

Ulrich Nowak Universität Heidelberg

Institut für Angewandte Mathematik

Im Neuenheimer Feld 293

D-6900 Heidelberg

W. Germany

- 1. Name of program or package: GRIDPACK
- 2. Descriptive title: Grid manipulation software
- 3. Problem domain: Problems described on grids, mainly derived from partial differential boundary value problems.
- **4. Method of solution:** Any grid-oriented method. (The package is most useful for implementing multigrid solutions, especially for general domains).
- 5. Programming language: Standard FORTRAN only.
- 6. Precision: mixed

- 7. Portability: Software developed on IBM, fully portable. (Machine-dependent constants are fully specified).
- 8. Other packages required: None
- 9. Mode of use: Collection of subroutines
- 10. Test or demonstration program available? Yes.
- 11. Length of code in lines: 20,000 Percentage comments: 15%
- 12. Special features: Requires secondary storage for some parts.
- 13. Documentation and references:

Detailed header comments? Yes.

User guide or manual, technical reports, papers, books: Manual on the same tape. General description in Chapter 4 of: A. Brandt, Multilevel adaptive techniques (MLAT) for partial differential equations: ideas and software, Mathematical Software III (John R. Rice, ed.), Academic Press 1977, pp. 273-314.

- 14. Approximate cost of obtaining software: None.
- 15. Restrictions on use: None.
- **16. Distributor:** Department of Applied Mathematics The Weizmann Institute of Science

Rehovot, Israel 76100

Attention: Dr. Dan Ophir

17. Original source of software:

Developer: Achi Brandt and Dan Ophir.

Institution: Weizmann Institute of Science, Rehovot, Israel, 76100.

Sponsor: ARO

18. For further information contact: Dr. Dan Ophir

Department of Applied Mathematics The Weizmann Institute of Science

Rehovot, Israel 76100

Telephone: (Country code 972) 54-83545

(Secretary)

- 1. Name of program or package: KUB | K
- 2. Descriptive title: Finite and infinite element mesh generator.
- 3. Problem domain: 2- and 3- dimensional domains of any degree of complexity.
- 4. Method of solution: Divide and conquer. Sparse matrix techniques are used throughout and a sparse mesh connectivity matrix is provided.
- 5. Programming language: FORTRAN IV.
- 6. Precision: Single.

- 7. Portability: IBM-360; IBM-370; VAX-11; CDC-6600; CDC-7600; XEROX-SIGMA-7. Easily portable to other machines.
- 8. Other packages required: None.
- 9. Mode of use: A main program calls the subroutines as required by the commands issued by user.
 10. Test or demonstration program available? Yes
- 11. Length of code in lines: 4500.

Percentage comments: 20.

- 12. Special features: The program is segmented for overlay. Secondary storage is optional.
- 13. Documentation and references:

Detailed header comments? No.

User guide or manual, technical reports, papers, books:

- a. User Manual and Operation Manual are provided with program.
- b. S. Pissanetzky. Int.J.Num.Meth.Engng. 17, 255-269 (1981).
- c. S. Pissanetzky. Brookhaven National Lab. Report BNL 27073 (1979).
- d. S. Pissanetzky. Computer Physics Communications, to appear.
- 14. Approximate cost of obtaining software: None. Write to liaison officer.
- 15. Restrictions on use: Only for research purposes.
- 16. Distributor: Liaison officer is Sergio Pissanetzky, Centro Atómico Bariloche, 8400 - Bariloche, R.N., Argentina.
- 17. Original source of software:

Developer: Sergio Pissanetzky

Institution: Comisión Nacional de Energía Atómica. Comisión Nacional de Energía Atómica. Sponsor:

18. For further information contact: Ronald Peierls, Chairman.

Applied Mathematics Department. Brookhaven National Laboratory. Upton, N.Y. 11973, U.S.A.

1. Name of program or package: ELLPACK

2. Descriptive title:

Solution of Elliptic Problems in 2 and 3 Dimensions

3. Problem domain: Linear, Second Order Elliptic PDEs. General domains in 2-D, rectanglar

domains in 3-D.

4. Method of solution:

Manifold

5. Programming language:

Fortran, has own language as Fortran preprocessor

6. Precision: Single or double

7. Portability:

High

8. Other packages required: None

9. Mode of use: Batch

10. Test or demonstration program available? Yes

11. Length of code in lines:

Percentage comments:

unknown, but reasonable

60-80,000

12. Special features: Included are: 4 YALE PACK sparse matrix programs, ACM Algorithm 533:NSPIV (Sparse Gauss elimination with pivoting), 7 ITPACK iterative method routines and 4 band solvers.

13. Documentation and references: Yes Detailed header comments? Solving Elliptic Problems with ELLPACK User guide or manual, technical reports, papers, books: J.R. Rice and R.F. Boisvert, Springer-Verlag, 1983. Several technical reports also available.

- 14. Approximate cost of obtaining software: \$75 (obsolete version), \$1000 (current
- 15. Restrictions on use:
- 16. Distributor: IMSL (obsolete version), Purdue Univ. (current version)

17. Original source of software: ELLPACK cooperative project

Developer: John R. Rice coordinator, about 20 contributors

Institution: Purdue University

Many Sponsor:

18. For further information contact: John R. Rice

Math Science 428 Purdue University W. Lafayette, IN 47907

(317)494-6007

1. Name of program or package: FISHPAK

2. Descriptive title: Efficient FORTRAN subprograms for solving separable elliptic equations

3. Problem domain: Separable elliptic equations subject to standard boundary conditions

4. Method of solution: Cyclic reduction and Fourier analysis

5. Programming language: ANSI FORTRAN

6. Precision: Single

7. Portability: PFORT verified

8. Other packages required: None

9. Mode of use: Subprograms

10. Test or demonstration program available? Yes, included with package 11. Length of code in lines: 20,000 Percentage comments: 30%

12. Special features: None

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

Algorithm 541, efficient FORTRAN subprograms for the solution of separable elliptic partial differential equations, TOMS, Vol. 5, No. 3, 1979

14. Approximate cost of obtaining software: \$300

15. Restrictions on use: None

16. Distributor: Scientific Computing Division

National Center for Atmospheric Research P.O. Box 3000, Boulder, Colorado 80307

17. Original source of software:

Developer: Paul N. Swartztrauber and Roland A. Sweet

Institution: NCAR Sponsor: NSF

18. For further information contact:

To order FISHPAK contact Sue Long, NCAR (303) 494-5151 Ext. 505 or FTS 322-5505. Questions should be directed to authors listed in 17.

Paul N. Swartztrauber: (303) 494-5151, Ext. 605 or FTS 322-5605.

Roland A. Sweet: (301) 921-3395 or FTS 921-3395.

1. Name of program or package: HELM3D

2. Descriptive title: Algorithm for Solving the Helmholtz Equation for the

Dirichlet Problem

3. Problem domain: General bounded three-dimensional regions

4. Method of solution: Capacitance matrix

5. Programming language: FORTRAN

6. Precision: Single

7. Portability: Easily portable

8. Other packages required: None

9. Mode of use: Callable subroutine

10. Test or demonstration program available? Yes

11. Length of code in lines: Approx. 1700 Percentage comments: 50

12. Special features: None

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

"Capacitance matrix methods for the Helmholtz equation on general three dimensional regions", MATH. COMP. 33(1979) 849-879.

"Algorithm 572", ACM Transactions on Math. Software, 7(1981) 239-246.

- 14. Approximate cost of obtaining software: \$50
- 15. Restrictions on use:
- 16. Distributor: ACM Algorithms Distribution Service

IMSL

Sixth Floor, NBC Building, 7500 Bellaire Blvd

17. Original source of sortware: 77036

Developer: Dianne P. O'Leary and Olof Widlund Institution: University of MI Courant Inst.

Sponsor: NSF, ERDA

18. For further information contact: Dianne P. O'Leary

Computer Science Department University of Maryland College Park, MD 20742 1. Name of program or package: HELM

2. Descriptive title: Solution of Helmholtz equation in a general two-dimensional domain

3. Problem domain: $-u_{xx}-u_{yy}+cu=f(x,y)$ in $\Omega \subseteq (0, 1) \times (0,1)$

u(x,y)=g(x,y) on $\Gamma = \partial\Omega$

4. Method of solution: Multi-grid iteration

5. Programming language: FORTRAN

6. Precision: Single

7. Portability: Developed on CDC 72/76

8. Other packages required: None

9. Mode of use: Sequence of subroutines to be called

10. Test or demonstration program available? $_{No}$

11. Length of code in lines: about 350 Percentage comments: 0%

12. Special features: Arrays on LEVEL 2 used

13. Documentation and references:

Detailed header comments? No

User guide or manual, technical reports, papers, books:

Programme list with some comments in report (German)

- 14. Approximate cost of obtaining software: Mailing costs
- 15. Restrictions on use: -
- 16. Distributor: Same as 18.

17. Original source of software:

Developer: W. Hackbusch

institution: Universität zu Köln

Sponsor:

18. For further information contact:

W. Hackbusch Institut für Informatik Universität Kiel Olshausenstr 40-60 D-2300 Kiel 1 Germany 1. Name of program or package: RECTCF

2. Descriptive title: Solution of elliptic second order problems in

a rectangle

3. Problem domain: PDE: $au_{xx}+bu_{xy}+cu_{yy}+du_x+eu_y+fu=g$, a=a(x,y), b=...

Boundary condition: Dirichlet, Neumann, mixed, periodic on rectangle

4. Method of solution: Iterative solution by a multi-grid method

Programming language: FORTRAN (equivalent programme available in ALGOL)

6. Precision: Single

7. Portability: Developed on CDC 72/76, easily portable

8. Other packages required: None

9. Mode of use: Sequence of subroutines to be called

10. Test or demonstration program available? Report contains test examples with output

11. Length of code in lines: about 500 Percentage comments: 0%

12. Special features: Arrays on LEVEL 2 used

13. Documentation and references:

Detailed header comments? None

User guide or manual, technical reports, papers, books:

The report "W. Hackbusch: A multi-grid method applied to a boundary value problem with variable coefficients in a rectangle. Report 77-17, 1977" describes the use of the programme and contains test examples.

- 14. Approximate cost of obtaining software: Mail costs
- 15. Restrictions on use: None
- 16. Distributor: Same as 18; or: OECD-NEA Data Bank

17. Original source of software:

Developer: W. Hackbusch

Institution: Universität zu Köln

Sponsor:

18. For further information contact:

W. Hackbusch Institut für Informatik Universität Kiel Olshausenstr. 40-60, D-2300 Kiel 1 Germany

1. Name of program or package:

IMSL TWODEPEP

2. Descriptive title:

Two dimensional partial differential equation solver

3. Problem domain:

General elliptic, parabolic and eigenvalue PDE systems in general 2-D regions

4. Method of solution:

Finite element method with quadratic, cubic or quartic triangular elements

5. Programming language:

FORTRAN

6. Precision:

Single and double for 32 bit computers; otherwise single only 7. Portability: Versions tested on IBM, CDC, DEC10, VAX, Data General, Burroughs, Univac,

Honeywell, Prime, Siemens and Cray computers 8. Other packages required:

9. Mode of use: -

Preprocessor reads input in special simple format

10. Test or demonstration program available? Yes

11. Length of code in lines:

Percentage comments:

12. Special features:

Has out of core solution capability using disk storage but also runs efficiently in a virtual memory environment.

13. Documentation and references:

Detailed header comments? No

User guide or manual, technical reports, papers, books:

IMSL TWODEPEP User's Manual (approx. 100 pages)

- 14. Approximate cost of obtaining software: \$1,500/year (\$900 for universities)
- 15. Restrictions on use: license agreement
- 16. Distributor: IMSL, Inc.

7500 Bellaire Blvd., 6th floor tele: (713) 772-1927

Houston, TX 77036

17. Original source of software:

Developer: Granville Sewell

Institution: IMSL

Sponsor:

18. For further information contact:

Granville Sewell

IMSL (tele: (713) 772-1927)

1. Name of program or package: PDE2D

2. Descriptive title: Nonlinear PDE Solver

3. Problem domain: Second Order Quasi-linear Homogeneous PDE's in

Two Space Variables

4. Method of solution: Conjugate Gradient, SOR

5. Programming language: 1956 ANSI FORTRAN

6. Precision: Single

7. Portability: Satisfies PFORT Standard of Portability

8. Other packages required: None

9. Mode of use: Callable Subroutines

10. Test or demonstration program available? Yes

11. Length of code in lines: 5000 Percentage comments: 70

12. Special features: None

13. Documentation and references:

Detailed header comments? Yes

User guide or manual, technical reports, papers, books:

"A Portable Software Package for Nonlinear Partial Differential Equations" ORNL/CSD-102

- 14. Approximate cost of obtaining software: None
- 15. Restrictions on use: None
- 16. Distributor: Robert Renka, Union Carbide Corporation, Nuclear Division

P. O. Box X, Building 4500N, D-224

Oak Ridge, TN 37830, Phone: (615) 576-5139

17. Original source of software:

Developer: Robert Renka

Institution: Oak Ridge National Laboratory

Sponsor: DOI

18. For further information contact:

Robert Renka

Union Carbide Corporation, Nuclear Division

P. O. Box X, Building 4500N, D-224

Oak Ridge, TN 37830 Phone: (615) 576-5139

Appendix A

SPARSE MATRIX 1982: SOFTWARE CATALOG

In conjunction with the Sparse Matrix Symposium to be held at Fairfield Glade, Tennessee on October 25-27, 1982, we are compiling a catalog of sparse matrix software. The purpose of the catalog is to help potential consumers or developers of sparse matrix software determine what software is available and how it can be obtained. All developers of sparse matrix software are invited to submit a one-page description of each program or package for inclusion in the catalog, which will be distributed to attendees at the conference; the catalog will be available to others on request subsequent to the conference. The catalog will include software for solving general sparse problems in the basic areas of linear systems; eigenvalues and least squares; in other general areas where sparse matrix problems are fundamental, such as optimization and differential equations; and in application areas where the use of sparse matrix techniques is critical.

To achieve a consistent format for the reporting of software, we have devised a form to be completed, together with guidelines and sample responses. This form must be completed with a typewriter using black ribbon. To further enhance reproduction quality of the catalog, please use only original forms, not copies. If additional forms are needed, please request more originals.

To help in organizing and indexing the catalog, we have also prepared an outline of various sparsematrix problem categories, printed on the back of the form. Please indicate which category and keywords apply to your software.

Select the single category that most closely describes the problem to be solved by your software and mark the most appropriate keyword on each line when applicable. This selection will determine the placement of your form in the catalog. An index will also be compiled, based on the methods indicated in Item 4 of the form. We have not listed separate keywords for complex matrices in Categories 1 and 2. If your code is for complex matrices, use the equivalent keywords for real matrices (e.g., "symmetric" for "hermitian").

Our goal is to make the software catalog as inclusive as possible. However, we reserve the right to reject a given submission if it appears to make no significant use of sparse matrix techniques. For example, a stiff ODE solver that provides for a sparse Jacobian matrix would be suitable for inclusion, whereas the average general ODE solver probably would not.

Please return the completed forms by July 1, 1982 and direct all correspondence to:

Robert C. Ward Union Carbide Corporation Nuclear Division P.O. Box Y Oak Ridge, TN 37830

Appendix B

INSTRUCTIONS AND SAMPLE RESPONSES FOR FORM

- Name of program or package: One word (typically 6 to 8 characters) name of package or
 of primary subroutine.
- 2. Descriptive title: Short phrase such as "Sparse linear system solver" or "Structural analysis package"
- 3. Problem domain: Specify problem(s) solved in as much generality as is warranted (e.g., unsymmetric linear systems, symmetric positive definite linear systems, reordering equations to minimize storage, etc.) or a specific application such as power network optimization.
- 4. Method of solution: Brief indication of methods used (e.g., SOR, bandwidth minimization, minimum degree ordering, Lanczos method, orthogonalization, simplex method, branch and bound, etc.)
- 5. Programming language: FORTRAN, Algol, PL/1, Basic, etc. Be more specific, if desired and appropriate (e.g., ANSI FORTRAN, FORTRAN IV, IBM FORTRAN H, etc.). If any assembly language modules are used, specify machine.
- 6. Precision: Single, double, both, mixed, etc.

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- 7. Portability: Specify machine(s) on which software was developed and state whether it is easily portable to other machines.
- 8. Other packages required: BLAS, LINPACK, EISPACK, IMSL, NAG, etc.
- 9. Mode of use: Callabie subroutine, stand-alone main program, etc.
- 10. Test or demonstration program available? Yes or no
- 11. Length of code in lines: (Approximate number.) Percentage comments: Approximate percentage of lines which are comments.
- 12. Special features: Does the software utilize any special features of computer architecture or storage, especially in handling very large problems? (e.g., the program permits or requires use of secondary storage, is easily segmented for overlay, is designed for efficiency in a paging environment, takes advantage of pipeline, parallel or array processors, etc.)
- 13. Documentation and references:
 - **Detailed header comments?** Yes, if sufficient to run program on straightforward problem, otherwise no.
 - **User guide or manual, technical reports, papers, books:** List only items of direct relevance to the use of the code or to the explanation of its theoretical basis.
- 14. Approximate cost of obtaining software: If fee is not a one-time charge, state time period covered (typically one year).
- 15. Restrictions on use: None, proprietary, license agreement required, etc.
- **16. Distributor:** List name, address and phone number of agency (e.g., NESC), commercial vendor, developer, etc., from which software may be obtained. Include electronic mail addites if software is obtainable via a computer network.
- 17. Original source of software:
 - **Developer:** List principle author(s) of software
 - **Institution:** University, laboratory, private company, etc. where software was developed **Sponsor:** Funding agency (DOE, NSF, ONR, ARO, AFOSR, etc.), corporation or institution which financed research and development
- 18. For further information contact: List name, address and phone number of one person, not necessarily a developer, who is willing to answer questions about software. Include FTS or other special communications network number if applicable.

Appendix C

CATEGORIES AND KEY WORDS

1. Systems of Linear Equations

real / complex nonsymmetric / symmetric indefinite / symmetric positive definite general sparse / band or profile oriented direct method / iterative method / combined or semi-iterative

2. Eigenvalue Problems

real / complex nonsymmetric / symmetric standard / generalized / lambda-matrix matrix required / only matrix-vector multiply required

3. Least Squares and other Approximations

norm: L₁ / L₂ / L₈ / other
matrix input by user / matrix generated by program from model
model: user defined / polynomial / spline / exponential / trigonometric / other
parameters: linear / separable / nonlinear
method: exchange / Ip / elimination / orthogonalization / other

4. Optimization

Mathematical programming:
objective: linear / separable / sum of squares / quadratic / nonlinear
constraints: none / bounds / linear / nonlinear

Combinatorial optimization and graph algorithms: integer programming / network flow / shortest path / minimal spanning tree / strongly connected components / other

5. Differential Equations

ODE / PDE finite differences / finite elements time dependent / time independent initial value problems / boundary value problems / both / mixed

6. Applications

structural analysis
electric power systems
image enhancement and reconstruction
petroleum and mineral prospecting and recovery
economic, energy and environmental modeling
statistical analysis
control theory and sensitivity analysis
other (specify):

Appendix D

The Harwell Subroutine Library

We wish the subroutine library to be of use to many people and we are willing to provide copies in source code of individual routines or of the whole library to external users on request. Charges are made (see below) to external users to cover the cost of handling, postage and documentation involved in fulfilling their requests for copies.

The charges cover only the copying and despatching of library routines. Therefore we do not undertake to provide any assistance that may be needed to use a subroutine successfully, and we do not guarantee the efficacy of any subroutine or documentation. However we hope that deficiences in subroutines and the documentation will be brought to our attention, in order that we can improve the library.

Except for a small number of subroutines obtained from elsewhere, the subroutines in the Harwell Subroutine Library are the property of the United Kingdom Atomic Energy Authority and a potential user must accept and abide by the conditions listed below. All communication with the library by external users should be made through Mr.S.Marlow, Building 8.9, AERE Harwell, Didcot, Oxon, OX11 ORA, England. (Tel. Abingdon 24141 ext. 2930), who is the liaison officer for the library's external affairs.

The conditions attached to external use are as follows:

- (i) the subroutines may only be used for research purposes by the person or organisation to whom they are supplied. They may not be copied for use by other persons or organisations, except with the written permission of the liaison officer.
- (ii) due acknowledgement is made of the use of subroutines in any research publications resulting from their use.
- (iii) the subroutines may be modified for use in research applications by external users. The nature of such modifications should be indicated in writing for information to the liaison officer. At no time however, shall the subroutines or modifications thereof become the property of the external user.
- (iv) the use of the subroutines in commercial applications must be agreed in writing with AERE Harwell and on terms and conditions to be negotiated. In the first instance, anyone considering such commercial applications should write to the liaison officer.

Conditions (i) and (iv) will be waived for most subroutines dating from before January 1977 and for some more recent ones. The conditions are listed under the subroutine entries in the current version of the catalogue.

The charges for library material are listed below. Overseas customers are charged on a different scale than that used for U.K. customers to cover the extra costs in meeting their requirements and all items are despatched by air mail. Charges to customers in the United Kingdom are subject to VAT. All prices given are valid to the 31st December 1982, and subject to review thereafter.

(1) Listings of subroutines

U.K.(excluding VAT) £7 each
Overseas £14 each

(2) Card decks of subroutines

U.K.(excluding VAT) £7 per 400 cards (minimum order £14)

Overseas £21 per 400 cards (minimum order £42)

(3) Subroutines on magnetic tape (including the cost of the tape which we supply)

U.K.(excluding VAT) £30 for the first two subroutines plus £2 for each subroutine in excess of two.

Overseas £50 for the first two subroutines plus £2 for each subroutine in excess of two.

(4) Complete library on tape (including the cost of the tape which we supply and one set of specification sheets)

U.K.(excluding VAT) £120 Overseas £200

(5) Additional complete sets of specification sheets

U.K.(excluding VAT) £30 each set Overseas £45 each set

Author Index

Bader, G.	111	Hackbusch, W.	117, 118
Barker, V. A.	30	Hanson, R. H.	75
Bartels, R. H.	88	Hanson, R. J.	89
Bennett, L. F.	<i>17</i> , 78	Harms, U.	2, 19
Boisvert, R. F.	114	Heath, M.	74
Brandt, A.	112	Hellerman, E.	92
Buckley, A.	97	Hiebert, K. L.	89
Bunch, J. R.	39	Hindmarsh, A. C.	107, 108
Calahan, D. A.	34, 35, 40,	Horton, S.	38
	41, 56	Houbak, N.	110
Calamai, P. H.	102	Jacobs, D. A. H.	65, 66, 68,
Coleman, R.	36, 37, 50,		69, 70, 71,
	52, 59, 91		72
Coleman, T. F.	101	Jensen, P. S.	20, 80
Conn, A. R.	102	Kaufman, L.	29
Cox, M.	53, 54	Keast, P.	43, 44, 45
Cox, R. L.	109	Kincaid, D. R.	58
Crane, H. L.	18	King, I. P.	18
Cullum, J.	81, 82	Lewis, J. G.	18, 51
Curtis, A. R.	7, 99, 106	Liu, J.	47, 51
de Boor, C.	42	Manteuffel, T. A.	60
Dembo, R.	105a	Markham, G.	67
Deuflhard, P.	111	Marsten, R.	90
Diaz, J. C.	43, 45	McNamee, J. M.	1, 2
Dillinger, W. H.	75	Meeraus, A.	105
Dodson, D. S.	6	Moler, C. B.	39
Dongarra, J. J.	39	More, J. J.	101
Drud, A.	105	Munksgaard, N.	63
Duff, I. S.	10, 14, 16,	Murtagh, B. A.	98
	17, 22, 23,	Neves, K. W.	6
	24, 25, 26,	Ng, E.	47, 74
	27, 46, 83,	Nielsen, H. B.	73
	100	Nikolai, P. J.	87a
Eisenstat, S. C.	48, 64	Nowak, U.	111
Elman, H. C.	64	O'Leary, D. P.	116
Ericsson, T.	86	Ophir, D.	112
Eriksson, J.	103	Paige, C. C.	61, 76
Fairweather, G.	43, 44, 45	Parlett, B. N.	84
Fletcher, R.	95	Pissanetzky, S.	3, 113
Garbow, B. S.	79, 101	Poole, W. G.	18
Gay, D. M.	92	Powell, M. J. D.	96, 99, 100
George, A.	47, 51, 74	Rarick, D. C.	92
Gibbs, N. E.	18	Reeves, C. M.	95
Giles, J. E.	93	Reid, J. K.	7, 11, 16,
Golub, G. H.	88		25, 27, 46,
Grimes, R. G.	58		55, 83, 84,
Gursky, M. C.	48		88, 94, 99
Gustavson, F. G.	4, 8, 13,	Reinsch, C.	79
	15, 32, 33,	Renka, R.	120
	49	Respess, J. R.	58

Rice, J. R.	114
Ruhe, A.	86
Rutishauser, H.	83
Saunders, M. A.	61, 76, 93,
	98
Schaumburg, K.	31
Schultz, M. H.	48, 64
Scott, D. S.	85
Sewell, G.	119
Sherman, A. H.	28, 48, 108
Smith, B. T.	79
Stadtherr, M. A.	38a
Stewart, G. W.	39
Stockmeyer, P. K.	18
Swartztrauber, P. N.	21, 115
Sweet, R. A.	115
Szyld, D. B.	5, 9, 12,
•	104
Tarjan, R.	16
Tarvestad, L.	57
Thomsen, P. G.	30, 110
Toint, P. L.	100
van der Vorst, H.	62
van Kats, J.	62
Vishnepolsky, O.	5, 9
Wasniewski, J.	31
Weiss, R.	42
Westerberg, A. W.	11
Widlund, O.	116
Wilkinson, J. H.	79
Willoughby, R. A.	81, 82
Wisniewski, J. A.	87
Wood, E. S.	38a
Yip, E.	38
Young, D. M.	58
Zlatev, Z.	30, 31, 73
•	

Software Index

		EA12	83
Algorithm 408	1*, 2	EA12	83
Algorithm 508	18	EA13	84
Algorithm 509	18	EA14 ECTLIB	38
Algorithm 529	16	EISPACK	60, 79*, 81, 87,
Algorithm 533	28, 114	EISPACK	87a
Algorithm 538	87a	ELLDACK	114
Algorithm 541	115	ELLPACK EPO1	103
Algorithm 546	42		80
Algorithm 572	116	EZ-GAL	22
Algorithm 575	14	F01BRF	23
Algorithm 582	18	F01BSF	53
Algorithm 583	76	F01MCF	24
APMATH64	36, 37, 50, 52,	F04AXF	54
	57, 59, 91	F04MCF	
ARCECO	43	FA01	83, 84
BCG25	65	FACSIMILE	106
BCG37	66	FFTPACK	21
BCGS	67	FISHPAK	115
BES	80	FM01	55, 83, 94
BKSLVE	32, 49	FM02	83, 95
BLAS	6, 39, 60, 61,	FULL ASSIGN	13
	64, 76, 87, 89	GEARBI	107
BLMAIN	81	GNSO	33
BLTF	15	GPSKCA	18
CCG25	65	GPSKRA	18
CCG37	66	GRIDPACK	112
CCGS	67	HALFP	4, 8*
CG25	65	HELM	117
CG37	66	HELM3D	116
CGS	67	ICCG	62
COLROW	45	ITPACK	58*, 114
CONOPT	105	KUBIK	113
CSFS	52	LA05	88*, 89, 90
CSPARSPAK	51	LARKIN	111
CUFS	37	LASO2	85
D03EBF	69	LASSO	75
D03ECF	70	LINPACK	39*, 87, 104
D03UAF	71 ,	LLSS01	73
D03UBF	72	LMAIN	82
DI205	68	LSOD28	109
DI209	68	LSODES	108
DI213	68	LSQR	76
DI3707	68	LVMAIN	82
DMGASP	20	MA15	55
DSM	101	MA17	94

[•] Indicates principal entry, if any, in cases of multiple entries.

MA27	46	RSFS	50
MA28	25*, 104, 109	RUFS	36
MA30	25	SIMITZ	87a
MA31	63	SIMPLE	91
MA32	26	SITSOL	59
MC09	94	SKYSOL	57
MC13	16*, 17, 25, 92	SMULT	4
MC19	7	SOLVEBLOK	42
MC20	11*, 25, 88	SPAR/BL	41
MC21	14*, 17, 25, 92	SPAR/SC	35
MC22	10*, 25	SPAR/VECTOR	34
MC23	17*, 25	SPARKS	110
MC24	25, 27*	SPARSE	2
ME22	10	SPARSPAK	47*, 51, 74, 75
ME23	17	SPARSPAK-B	74
ME24	27	SPAR2PAS	38a
ME27	46	SPLP	89
ME28	25	SPRSBLAS	6
ME30	25	SSLEST	30*, 110
MFLPP	102	STLM	86
MINOS	93, 98*	SUBMAT	12
NLPNET	105a	SYMFAC	32, 49
NS03	94	SYMMLQ	61
NSPFAC	28	TCHLIB	60
NSPIV	28, 114	TD02	94, 99*
NUMFAC	32, 49	TD03	100
P3	92	TRACMN	87
P4	92	TRANS	9
PCGPAK	64	TWODEPEP	119
PDE2D	120	URAND	87
PORT	29	VA08	95
PROD	5	VA14	96
PROFILE/S	56	VE05	97
PROFILE/U	40	VMSYST	20*, 80
RALAPAĆK	3	XERROR	89
RECTCF	118	XMP	90
RNCLIN	77	Y12M	31
RNRWIN	78	YSMP	48*, 108, 114
ROWCOL	44		